

# SPIN SQUEEZING AND OTHER ENTANGLEMENT TESTS FOR TWO MODE SYSTEMS OF IDENTICAL BOSONS

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## Abstract

The concept of entangled quantum states is considered in the context of systems of identical particles, based on the requirement that in order to represent physical states both for the overall system and the sub-systems which may be entangled, the density operators must satisfy the symmetrisation principle and conform to super-selection rules that prohibit states in which there are coherences between differing total particle numbers. These requirements, their justification and recent challenges to them are fully discussed in the paper. In the second quantisation approach used in this paper, both the system and the sub-systems are modes (or sets of modes) rather than particles, particles being associated with different occupancies of the modes. The definition of entangled states is based on first defining the non-entangled states - after specifying which modes constitute the sub-systems that may or may not be entangled, entanglement being a relative concept. Although multimode systems are also considered, this paper is mainly focused on two mode entanglement for massive bosons, such as bosonic atoms, but the results also apply for photons. A number of inequalities involving variances and mean values of operators based on the mode annihilation and creation operators have been proposed as tests for two mode entangled states, including the inequalities that define spin squeezing - the spin operators are bilinear combinations of the mode operators. The criteria for spin squeezing in two mode systems is examined, and it is found that spin squeezing is best considered for principle spin operator components, where the covariance matrix defining the spin fluctuations is diagonal. The modes related to the principle spin components are then orthonormal linear combinations of the original ones. It is shown that the presence of spin squeezing in at least one of the spin components requires entanglement of the relevant pair of modes. The paper also considers several of the other proposed tests for entanglement, including ones based on the sum of the variances for two spin components. However, whilst all of the tests are still valid when the present concept of entanglement based on the symmetrisation and super-selection rule criteria is applied, additional tests have been obtained here. Sometimes the new tests are less stringent than those obtained in other papers. In one case where the link between spin squeezing and entanglement was based on a concept of entanglement which is inconsistent with the symmetrisation principle, a revised treatment with modes rather than identical particles as the sub-systems does lead to spin squeezing being a test of entanglement if the sub-systems are pairs of modes - each pair however only being associated with a single boson.

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# 1 Introduction

Since the work of Einstein et al [1] on local realism, the famous cat paradox of Schrodinger [2] and the derivation by Bell et al [3], [4] of inequalities based on treating measured quantities via a classical hidden variable theory which certain quantum quantum systems violated, *entanglement* has been recognised as being one of the key features that distinguishes quantum physics from classical physics. It arises in the context of quantum systems composed of distinct components or *sub-systems*. Such sub-systems are usually associated with sub-sets of the physical quantities applying to the overall system, and in general more than one choice of sub-systems can be made. The formalism of quantum theory treats *pure states* for systems made up of two or more distinct sub-systems via tensor products of sub-system states, and since these product states exist in a Hilbert space, it follows that linear combinations of such products could also represent possible pure quantum states for the system. Such *quantum superpositions* which cannot be expressed as a *single* product of sub-system states are known as *entangled* (or *non-separable*) states. The concept of entanglement can also be extended to *mixed states*, where quantum states for the system and the sub-systems are specified by density operators. The detailed definition of entangled states is set out in Section 2. This definition is based on first carefully defining the *non-entangled* (or *separable*) states such that *all* non-entangled states must be possible physical states. The entangled states are then just the physical states which are not non-entangled states. The notion of *physical states*, the nature of the systems and *sub-systems* involved and the specific features required in the definition of non-entangled states when *identical particles* are involved is discussed in detail in Section 2. Entangled states underlie a number of effects that cannot be interpreted in terms of classical physics, including *spin squeezing*, non-local measurement correlations - such as for the Einstein-Podolski-Rosen (*EPR*) *paradox* and violations of *Bell Inequalities*. Recent expositions on the role of entanglement in these effects and more generally in quantum information science include [5], [6], [7], [8], [9], [10].

It is now generally recognised that entanglement is a *relative* concept ([11], [12], [13]), [7], [14], [15] and not only depends on the quantum state under discussion but also on which *sub-systems* are being considered as entangled (or non-entangled). A quantum state may be entangled for one choice of the sub-systems but may be non-entangled if another choice of sub-systems is made, an example being for the hydrogen atom [13] where energy eigenstates are non-entangled if the sub-systems refer to the centre of mass and the relative position of the electron from the proton, but which would be entangled if the sub-systems were the positions of the electron and proton. An example involving two different choices of single particle states in a two mode Bose condensate is given in Section 4.

For a general quantum state various *measures* of entanglement have been

defined - see [7], [8], [14], [15], [16], [17], [18], for details of these, and are aimed at quantifying entanglement to determine which states are more entangled than others. This is important since entanglement is considered as a resource needed in various *quantum technologies*, such as teleportation and quantum information processing. Calculations based on such measures of entanglement confirm that for some choices of sub-systems the quantum state is entangled, for others it is non-entangled. For two mode pure states the *entanglement entropy* - being the difference between the entropy for the pure state (zero) and that associated with the reduced density operator for either of the two sub-systems - is a useful entanglement measure. As entropy and information changes are directly linked [7], [8], this measure is of importance to *quantum information science*. Another entanglement measure is *particle entanglement entropy*, defined by Wiseman et al [19], [20], [16] for identical particle systems and based on projecting the quantum state onto states with definite particle numbers.

Although not directly relatable to the various quantitative measures of entanglement, the results for certain measurements can play the role of being *signatures* or *witnesses* or *tests* of entanglement [14], [15], [16]. These are in the form of *inequalities* for *variances* and *mean values* for certain physical quantities, which are consequent on the inequalities that would apply for non-entangled quantum states. If such inequalities are *violated* then it can be concluded that the state is *entangled* for the relevant sub-systems. It cannot be emphasised enough that these tests provide *sufficiency conditions* for establishing that a state is entangled. The failure of a test does *not* guarantee non-entanglement - sufficiency does not imply *necessity*. The violation of a *Bell inequality* is an example of such a signature of entanglement, and the demonstration of *spin squeezing* is regarded as another. However, the absence of spin squeezing (for example) does not guarantee non-entanglement, as the case of the *NOON* state in SubSection 4.3 shows. A significant number of such inequalities have now been proposed and such signatures of entanglement are the primary focus of the present paper, which is aimed at identifying which of these inequalities really do identify entangled states, especially in the context of *two mode* systems of *identical bosons*.

At present there is *no clear linkage* between quantitative measures of entanglement (such as entanglement entropy) and the quantities used in conjunction with the various entanglement tests (such as the relative spin fluctuation in spin squeezing experiments). Results for experiments demonstrating such non-classical effects cannot yet be used to say much more than the state *is* entangled, whereas ideally these experiments should determine *how* entangled the state is.

This paper deals with identical particles - bosons or fermions. In the *second quantisation* approach used here the system is regarded as a set of *quantum fields*, each of which may be considered as a collection of single particle states or *modes*. Hence both the system and sub-systems will be specified via the modes that are involved, so here the sub-systems in terms of which non-entangled (and hence entangled) states are defined are *modes* or *sets* of modes, not particles [11], [12], [13]), [7], [21], [22]. In this approach, *particles* will be described via the *occupancies* of the various modes, so that situations with differing numbers

of particles will be treated as differing quantum *states* of the same system, not as different systems - as in the *first quantisation* approach. Note that the choice of modes is *not unique* - original sets of orthogonal one particle states (modes) may be replaced by other orthogonal sets. An example is given in Section 3. Modes can often be categorised as *localised* modes, where the corresponding single particle wavefunction is confined to a restricted spatial region, or may be categorised as *delocalised* modes, where the opposite applies. Single particle harmonic oscillator states are an example of localised modes, momentum states are an example of delocalised modes. This distinction is significant when phenomena such as EPR violations and teleportation are considered.

Although *multi-mode* systems are also considered, in this paper we mainly focus on *two mode* systems of identical *bosonic* atoms, where the atoms at most occupy only two single particle states or modes. For bosonic atoms this situation applies in two mode interferometry, where if a single hyperfine component is involved the modes concerned may be two distinct spatial modes, such as in a double well magnetic or optical trap, or if two hyperfine components are involved in a single well trap each component has its own spatial mode. Large numbers of bosons may be involved since there is no restriction on the number of bosons that can occupy a bosonic mode. For fermionic atoms each hyperfine component again has its own spatial mode. However, if large numbers of *fermionic* atoms are involved then as the Pauli exclusion principle only allows each mode to accommodate one fermion, it follows that a large number of modes must be considered and two mode systems would be restricted to at most two fermions. Consideration of multi-mode entanglement for large numbers of fermions is *outside* the scope of the present paper (see [23] for a treatment of this), and unless otherwise indicated the focus will be on *bosonic modes*. Although oriented towards identical bosonic *atoms* the paper also applies to *photons*, though details of the analysis will differ.

The work presented here begins with the *fundamental issue* of how an entangled state should be *defined* in the context of systems involving *identical particles*. In the commonly used *mathematical approach* for defining entangled states, this requires *first* defining a general *non-entangled* state, all *other* states therefore being entangled. It is contended that the *density operators* both for the overall system states and for the sub-system states of non-entangled states must represent *physical states* and in some other work (discussed below) this is not the case. A key feature required of all physical states for systems involving identical particles, entangled or not is that they satisfy the *symmetrization principle*. This places restrictions both on the form of the overall density operator and also on what can be validly considered to be a sub-system. In particular this rules out *individual* identical particles being treated as sub-systems, as is done in some papers (see below). In addition, *super-selection rules* (SSR) [24] only allow density operators which have *zero coherences* between states with *differing total numbers* of particles to represent valid *physical states*, and this will be taken into account for all physical states of the overall system, entangled or not. This is referred to as the *global particle number super-selection rule*. In *non-entangled* or *separable* states the density operator is a sum over products

of sub-system density operators, each product being weighted by its probability of occurring (see below for details). For the non-entangled or separable states, a so-called *local particle number super-selection rule* will *also* be applied to the density operators describing each of the *sub-systems*. These sub-system density operators must then have zero coherences between states with differing numbers of *sub-system particles*. This additional restriction excludes density operators as defining non-entangled states when the sub-system density operators do not conform to the local particle number super-selection rule. Consequently, density operators where the local particle number SSR does not apply would be regarded as entangled states. This viewpoint is discussed in papers by Bartlett et al [25], [26] as one of several *operational approaches* for defining entangled states. However, other authors such as [27], [28] state on the contrary that states when the sub-system density operators do *not* conform to the local particle number super-selection rule *are* still separable, others such as [29], [30] do so by implication, so in this paper we are advocating a *revision* to the *widely held notion* of entanglement in identical particle systems, the consequence being that the set of entangled states is now much *larger*. This is a *key idea* in this paper - not only should super-selection rules on particle numbers be applied to the *overall* physical state, entangled or not, but it *also* should be applied to the density operators that describe states of the modal *sub-systems* involved in the general definition of *non-entangled* states. The reasons for adopting this viewpoint are set out below. Apart from the papers by Bartlett et al [25], [26] we are not aware that this definition of non-entangled states has been invoked previously, indeed the opposite approach has been proposed [27], [28]. However, the idea of considering sub-system states which satisfy the local particle number SSR has been presented in several papers - [27], [28], [25], [26], [31], [32], [33], mainly in the context of pure states for bosonic systems, though in these papers the focus is on issues other than the definition of entanglement - such as quantum communication protocols [27], multicopy distillation [25], mechanical work and accessible entanglement [31], [32] and Bell inequality violation [33]. The consequences for entanglement of applying this super-selection rule requirement to the sub-system density operators are quite *significant*, and in the present paper important *new entanglement tests* are determined. Not only can it immediately be established that spin squeezing *requires* entangled states, but though several of the other inequalities (see below) that have been used as signatures of entanglement are still valid, *additional tests* can be obtained which only apply to entangled states that are defined to conform to the symmetrisation principle and the super-selection rules.

It is worth emphasising that requiring the sub-system density operators satisfy the local particle number SSR means that there are less states than otherwise would be the case which are classed as non-entangled, and *more states* will be regarded as *entangled*. It is therefore not surprising that additional tests for entanglement will result. If *further restrictions* are placed on the sub-system density operator - such as requiring them to correspond to a fixed number of bosons again there will be more states regarded as entangled, and even more entanglement tests will apply. A particular example is given in SubSection 5.3,

where the sub-systems are restricted to one boson states.

The *symmetrisation* requirement for systems involving identical particles is well established since the work of Dirac. There are two types of justification for applying the *super-selection rules* for systems of identical particles. The first approach is based on simple considerations and will be outlined here. The second approach is more sophisticated and involves linking the absence or presence of SSR to whether or not there is a suitable *reference frame* in terms of which the quantum state is described [34], [35], [36], [27], [28], [37], [38], [39], [26], [31], [32], [16]. This approach will be described in SubSection 2.7 and Appendix 11, the key idea being that SSR are a consequence of considering the description of a quantum state by an external observer (Charlie) whose phase reference frame has an *unknown phase difference* from that of an observer ((Alice) more closely linked to the system being studied. Thus, whilst Alice's description of the quantum state may violate the SSR, the description of the *same* quantum state by Charlie will not. In the main part of this paper the density operator  $\hat{\rho}$  used to describe the various quantum states will be that of the external observer (Charlie). Note that if the relationship between the phase references is *known*, then the SSR can be challenged (see SubSection 2.8 and Appendix 11). Returning to the more simple reasons referred to for invoking the superselection rule to exclude quantum superposition states with differing numbers of identical particles (both massive and otherwise), these may be summarised as:

1. No way is known for creating such states.
2. No way is known for measuring all the properties of such states, even if they existed.
3. Coherence and interference effects can be understood without invoking the existence of such states.
4. The stability of such states against decoherence processes may not be great, so even if they could be created, they could rapidly change to other states. However, decoherence time scales that are not too short would be acceptable, so this last reason is of lesser importance.

Invoking the physical existence of states that as far as we know cannot be made or measured, and for which there are no known physical effects that require their presence seems a rather unnecessary feature to add to the non-relativistic quantum physics of many body systems or to quantum optics, and considerations based on the general principle of simplicity (Occam's razor) would suggest not doing so until a clear physical justification for including them is found. Furthermore, experiments can be carried out on each of the mode sub-systems considered as a *separate* system, and essentially the *same reasons* that justify applying the super-selection rule to the overall system also apply to the separate mode sub-systems in the context of defining *non-entangled states*. Hence, unless it can be justified to ignore the super-selection rule for the overall system it would be *inconsistent* not to apply it to the sub-system as well. The *onus* is on those who wish to ignore the super-selection rule for the separate modes to justify why it is being applied to the overall system. In addition, *joint measurements* on *all* the sub-systems can be carried out, and the interpretation of the measurement probabilities requires the density operators for the sub-

system states to be physically based. The general application of super-selection rules has however been challenged (see SubSection 2.7) on the basis that super-selection rules are not a fundamental requirement of quantum theory, but are restrictions that could be lifted if there is a suitable system that acts as a *reference* for the coherences involved. In Section 2 and related Appendix 12 an analysis of these objections to the super-selection rule is presented, and in Appendix 11 we see that the approach based on phase reference frames does indeed justify the application of the SSR both to the general quantum states for multi-mode systems of identical particles and to the sub-system states for non-entangled states of these systems.

The other focus of this paper is on *spin squeezing*. Spin squeezing was first defined in the paper by Kitagawa et al [40] for general spin systems. It was suggested in this paper that correlations between the individual spins was needed to produce spin squeezing, though no quantitative proof was presented and the more precise concept of entanglement was not mentioned. For the case of two mode systems the earliest paper linking spin squeezing to entanglement is that of Sorensen et al [41], which considers a system of identical bosonic atoms, each of which can occupy one of two internal states. This paper states that spin squeezing requires the quantum state to be entangled, with a proof given in the Appendix. A consideration of how such spin squeezing may be generated via collisional interactions is also presented. The paper by Sorensen et al is often referred to as establishing the link between spin squeezing and entanglement - see for example Micheli et al [42], Toth et al [43], Hyllus et al [44]. However, the paper by Sorensen et al [41] is based on a definition of non-entangled states in which the sub-systems are the identical particles, and this is inconsistent with the symmetrization principle. The present paper establishes the link between spin squeezing and entanglement based on a definition of entanglement consistent with the system and sub-system density operators representing physical states.

It is also important to consider which *components* of the spin operator vector are squeezed, and this issue is also considered in the present paper. In the context of the present second quantisation approach to identical particle systems the three spin operator components for two mode systems are expressed in terms of the annihilation, creation operators for the two chosen modes. Spin squeezing can be defined (see Section 3) in terms of the variances of these spin operators, however the *covariance matrix* for the three spin operators will in general have off-diagonal elements, and spin squeezing is better defined in terms of rotated spin operators referred to as *principal spin operators* for which the covariance matrix is *diagonal*. The principal spin operators are related to new mode annihilation, creation operators in the same form as for the original spin operators, where the *new modes* are two orthogonal linear combinations of the originally chosen modes. In discussing the relationship between spin squeezing and entanglement, the modes which may be entangled are generally those associated with the definition of the spin operators.

The plan of this paper is as follows. In Section 2 the key definitions of entangled states are covered, along with detailed discussion on why the sym-



metrisation principle and the super-selection rule is invoked. Challenges to the necessity of the super-selection rule are outlined, with arguments against such challenges dealt with in Appendices 11, 12. and 13. The next Section 3 sets out the definitions of spin squeezing and in the following Section 4 it is shown that spin squeezing is a signature of entanglement, both for the principle spin operators with entanglement of the two new modes and for the original spin operators with entanglement of the original modes. A number of other tests for entanglement proposed by other authors are considered in Section 5, with details of these treatments set out in Appendices 14, 15, 16. Two key mathematical inequalities are derived in Appendix 9. The final Section 7 summarises and discusses the key results.

## 2 Entanglement

### 2.1 Physical States

The standard quantum theory notions of *physical systems* that can exist in various *states* and have associated *quantities* on which *measurements* can be made are presumed in this paper. The measuring system made be also treated via quantum theory, but there is always some component that behaves *classically*, so that quantum fluctuations in the quantity recorded by the *observer* are small. The term *physical state* refers to a state that can either be prepared via a process consistent with the laws of quantum physics and on which measurements can be then performed and the probabilistic results predicted from this state (*prediction*), or a state whose existence can be inferred from later quantum measurements (*retrodiction*). In quantum theory, physical states are *represented* by *density operators* for mixed states or *state vectors* for pure states, which must satisfy symmetrisation and other basis requirements in accordance with the laws of quantum theory. The quantum state, the system it is associated with and the quantities that can be measured are viewed here as entities that are viewed as being *both* ontological and epistimological. The observer is important, but there is actually something out there to be studied. In addition to those associated with physical states, other density operators and state vectors may be introduced for *mathematical* convenience. For physical states, the density operator is determined from either the preparation process or inferred from the measurement process, and in general it is a statistical mixture of density operators for possible preparation processes. Measurement itself constitutes a possible preparation process. Following preparation, further experimental processes may change the physical state and dynamical equations give the time evolution of the density operator between preparation and measurement, the simplest situation being where measurement takes place immediately after preparation. A full discussion of the predictive and retrodictive aspects of the density operator is given in papers by Pegg et al [45], [46]. Whilst there are often different mathematical forms for the density operator that lead to the same predictive results for subsequent measurements, applying the results of the measurements to retrodictively determines the *preferred form* of the density operator that is consistent with the *available* preparation and measurement operators. An example is given in [46].

### 2.2 Entangled and Non-Entangled States

#### 2.2.1 General Considerations

Here the commonly applied *mathematical approach* to defining entangled states will be described [8]. The formal definition of what is meant by an entangled state starts with the pure states, described via a vector in a Hilbert space. The formalism of quantum theory treats *pure states* for systems made up of two or more distinct sub-systems via tensor products of sub-system states  $|\Phi_A\rangle \otimes |\Phi_B\rangle \otimes |\Phi_C\rangle \dots$ . Such products are called *non-entangled* or *separable* states.

However, since these product states exist in a Hilbert space, it follows that linear combinations of such products of the form  $|\Phi\rangle = \sum_{\alpha\beta\gamma\dots} C_{\alpha\beta\gamma\dots} |\Phi_A^\alpha\rangle \otimes |\Phi_B^\beta\rangle \otimes |\Phi_C^\gamma\rangle \dots$  could also represent possible pure quantum states for the system. Such *quantum superpositions* which cannot be expressed as a *single* product of sub-system states are known as *entangled* (or *non-separable*) states.

The concept of entanglement can be extended to *mixed states*, which are described via density operators in the Hilbert space. If  $A, B, \dots$  are the sub-systems with  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  being density operators the sub-systems  $A, B, \dots$  then a *general non-entangled* or *separable* state is one where the overall density operator  $\hat{\rho}$  can be written as the weighted sum of tensor products of these sub-system density operators in the form

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes \dots \quad (1)$$

with  $\sum_R P_R = 1$  and  $P_R \geq 0$  giving the probability that the specific product state  $\hat{\rho}_R = \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes \dots$  occurs. *Entangled* states (or *non-separable* states) are those that cannot be written in this form, so in this approach knowing what the term entangled state refers to is based on *first* knowing what the general form is for a non-entangled state.

The alternative *operational approach* to defining entangled states focuses on whether or not they exhibit certain non-classical features such as Bell Inequality violation, or whether they can be used in various quantum information protocols, or even whether the states cannot be created via *local operations* and *classical communications* (*LOCC*). Such an approach is discussed by Bartlett et al (see [25], Section IIB). As will be seen in SubSection 2.9, the particular definition of entangled states based on their non-creatability via LOCC essentially coincides with the approach used in the present paper. On the other hand, Wiseman et al [47], [48] and Reid et al [10] discuss the concept of a *heirarchy* of *entangled states*, with states exhibiting *Bell nonlocality* being a subset of states for which there is *EPR steering*, which in turn is a subset of the *entangled states*, the latter being defined as states whose density operators cannot be written as in Eq. (1) though without further consideration if additional properties are required for the sub-system density operators. The operational approach could lead into a quagmire of differing interpretations of entanglement depending on which non-classical feature is highlighted, so the present mathematical approach is generally favoured [8]. It is also compatible with later classifying entangled states in a heirarchy.

### 2.2.2 Local Systems and Operations

As pointed out by Vedral [7], one reason for calling these states separable is associated with the idea of performing operations on the separate sub-systems that do not affect the other sub-systems. Such operations on such *local systems* are referred to as *local operations* and include unitary operations  $\hat{U}_A, \hat{U}_B$ , that

change the states via  $\hat{\rho}_R^A \rightarrow \hat{U}_A \hat{\rho}_R^A \hat{U}_A^{-1}$ ,  $\hat{\rho}_R^B \rightarrow \hat{U}_B \hat{\rho}_R^B \hat{U}_B^{-1}$ , etc as in a time evolution, and could include processes by which the states  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , are separately prepared from suitable initial states. We note that performing local operations on a separable state only produces another separable state, not an entangled state. Such local operations are obviously facilitated in experiments if the sub-systems are essentially *non-interacting* - such as when they are spatially *well-separated*, though this does not have to be the case. The local systems and operations could involve sub-systems whose quantum states and operators are just in different parts of Hilbert space, such as for cold atoms in different hyperfine states even when located in the same spatial region. Note the distinction between *local* and *localised*. If one observer (Alice) is associated with preparing separate sub-system  $A$  in a physical state  $\hat{\rho}_R^A$  via local operations with a probability  $P_R$ , a second observer (Bob) could be then advised via a *classical communication* channel to prepare sub-system  $B$  in state  $\hat{\rho}_R^B$  via local operations. The overall quantum state prepared by both observers via this local operation and classical communication protocol (*LOCC*) would then be the bipartite non-entangled state  $\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B$ . Multipartite non-entangled states of the form (1) can also be prepared via LOCC protocols involving further observers. As will be seen, the separable or non-entangled states are just those that can be prepared by LOCC protocols.

### 2.2.3 Mean Values and Correlations

For non-entangled states as in Eq. (1) the mean value for measuring a physical quantity  $\hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \dots$ , where  $\hat{\Omega}_A, \hat{\Omega}_B, \hat{\Omega}_C, \dots$  are Hermitian operators representing physical quantities for the separate sub-systems, is given by

$$\langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \dots \rangle = \sum_R P_R \langle \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B \rangle_R^B \langle \hat{\Omega}_C \rangle_R^C \dots \quad (2)$$

where  $\langle \hat{\Omega}_K \rangle_R^K = \text{Tr}(\hat{\Omega}_K \hat{\rho}_R^K)$ , ( $K = A, B, \dots$ ), is the mean value for measuring  $\hat{\Omega}_K$  in the  $K$  sub-system when its density operator is  $\hat{\rho}_R^K$ . Since the overall mean value is not equal to the product of the separate mean values, the measurements on the sub-systems are said to be *correlated*. However, for the general non-entangled state as the mean value is just the products of mean values weighted by the probability of preparing the particular product state - which involves a LOCC protocol, as we have seen - the correlation is *classical* rather than *quantum* [8]. In the case of a single product state where  $\hat{\rho} = \hat{\rho}^A \otimes \hat{\rho}^B \otimes \hat{\rho}^C \otimes \dots$  we have  $\langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \dots \rangle = \langle \hat{\Omega}_A \rangle^A \langle \hat{\Omega}_B \rangle^B \langle \hat{\Omega}_C \rangle^C \dots$  which is just the product of mean values for the separate sub-systems, and in this case the measurements on the sub-systems are said to be *uncorrelated*. For entangled states however the last result for  $\langle \hat{\Omega}_A \otimes \hat{\Omega}_B \otimes \hat{\Omega}_C \otimes \dots \rangle$  does not apply, and the correlation is strictly quantum.

### 2.2.4 Constraints on Sub-System Density Operators

A key issue however is whether density operators  $\hat{\rho}$  and  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , in Eq. (1) always represent possible *physical states*, even if the operators  $\hat{\rho}$  and  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , etc satisfy all the standard mathematical requirements for density operators - Hermitiancy, positiveness, trace equal to unity, trace of density operator squared being not greater than unity. In this paper it will be argued that there are further requirements not only on the overall density operator, but also on those for the individual sub-systems that are imposed by symmetrisation and super-selection rules.

## 2.3 Joint and Separate Measurements, Reduced Density Operator

### 2.3.1 Joint Measurements

Measurements can be carried out on all the sub-systems and the results expressed in terms of the *joint probability* for various outcomes. If  $\hat{\Omega}_A$  is a physical quantity associated with sub-system  $A$ , with eigenvalues  $\lambda_i^A$  and with  $\hat{\Pi}_i^A$  the projector onto the subspace with eigenvalue  $\lambda_i^A$ ,  $\hat{\Omega}_B$  is a physical quantity associated with sub-system  $B$ , with eigenvalues  $\lambda_j^B$  and with  $\hat{\Pi}_j^B$  the projector onto the subspace with eigenvalue  $\lambda_j^B$  etc., then the *joint probability*  $P_{AB..}(i, j, ..)$  that measurement of  $\hat{\Omega}_A$  leads to result  $\lambda_i^A$ , measurement of  $\hat{\Omega}_B$  leads to result  $\lambda_j^B$ , etc is given by

$$P_{AB..}(i, j, ..) = Tr(\hat{\Pi}_i^A \hat{\Pi}_j^B ... \hat{\rho}) \quad (3)$$

This joint probability depends on the full density operator  $\hat{\rho}$  representing the physical state as well as on the quantities being measured.

### 2.3.2 Non-Entangled States - Joint Measurements

In the case of the general *non-entangled state* we find that the joint probability is

$$P_{AB..}(i, j, ..) = \sum_R P_R P_A^R(i) P_B^R(j) .. \quad (4)$$

where

$$P_A^R(i) = Tr(\hat{\Pi}_i^A \hat{\rho}_R^A) \quad P_B^R(j) = Tr(\hat{\Pi}_j^B \hat{\rho}_R^B) \quad .. \quad (5)$$

are the probabilities for measurement results for  $\hat{\Omega}_A, \hat{\Omega}_B, ..$  on the separate sub-systems with density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , etc and the overall joint probability is given by the products of the probabilities  $P_A^R(i), P_B^R(j), ..$  for the measurement results  $\lambda_i^A, \lambda_j^B, ..$  for physical quantities  $\hat{\Omega}_A, \hat{\Omega}_B, ..$  if the sub-systems are in the states  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , etc. These products are then weighted by the probability  $P_R$  that the system is prepared in the particular product state  $\hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes ..$  to determine the overall joint probability  $P_{AB..}(i, j, ..)$ . The overall probability is of a *classical* form. Obviously this joint probability depends on the sub-system density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , etc.

### 2.3.3 Single Measurements and Reduced Density Operator

The *reduced density operator*  $\hat{\rho}_A$  for sub-system  $A$  given by

$$\hat{\rho}_A = Tr_{B,C,\dots}(\hat{\rho}) \quad (6)$$

and enables the results for measurements on sub-system  $A$  to be determined for the situation where the results for all joint measurements involving the other sub-systems are *discarded*. The probability  $P_A(i)$  that measurement of  $\hat{\Omega}_A$  leads to result  $\lambda_i^A$  irrespective of the results for measurements on the other sub-systems is given by

$$\begin{aligned} P_A(i) &= \sum_{j,k,\dots} P_{AB\dots}(i, j, \dots) = Tr(\hat{\Pi}_i^A \cdot \hat{\rho}) \\ &= Tr_A(\hat{\Pi}_i^A \hat{\rho}_A) \end{aligned} \quad (7)$$

using  $\sum_j \hat{\Pi}_j^B = \hat{1}$ , etc. Hence the reduced density operator  $\hat{\rho}_A$  plays the role of specifying the physical state for mode  $A$  considered as a separate sub-system, even if the original state  $\hat{\rho}$  is entangled.

For the general non-entangled state, the reduced density operator for sub-system  $A$  is given by

$$\hat{\rho}_A = \sum_R P_R \hat{\rho}_R^A \quad (8)$$

A key feature of a non-entangled state is that the results of a measurement on any *one* of the sub-systems is *independent* of the states for the *other* subsystems. From Eqs.(7) and (8) the probability  $P_A(i)$  that measurement of  $\hat{\Omega}_A$  leads to result  $\lambda_i^A$  is given by

$$P_A(i) = \sum_R P_R P_A^R(i) \quad (9)$$

where the reduced density operator is given by Eq. (8) for the non-entangled state in Eq. (1). This result only depends on the reduced density operator  $\hat{\rho}_A$ , which represents a state for sub-system  $A$  and which is a statistical mixture of the sub-system states  $\hat{\rho}_R^A$ , with a probability  $P_R$  that is the *same* for all sub-systems. The result for the measurement probability  $P_A(i)$  is just the statistical average of the results that would apply if sub-system  $A$  were in possible states  $\hat{\rho}_R^A$ . For all quantum states the final expression for the measurement probability  $P_A(i)$  only involves a trace of quantities  $\hat{\Pi}_i^A$ ,  $\hat{\rho}_A$  that apply to sub-system  $A$ , but for a non-entangled state the reduced density operator  $\hat{\rho}_A$  is given by an expression (8) that does *not* involve density operators for the other sub-systems. Thus for a non-entangled state, the probability  $P_A(i)$  is *independent* of the states  $\hat{\rho}_R^B$ ,  $\hat{\rho}_R^C$ , associated with the other sub-systems. Analogous results apply for measurements on the other sub-systems.

## 2.4 Bell Inequalities

### 2.4.1 Hidden Variable Theory

A key feature of entangled states is that they are associated with *violations of Bell inequalities* [3] and hence can exhibit this particular *non-classical* feature. The Bell inequalities arise in attempts to restore a *classical* interpretation of quantum theory via *hidden variable* treatments, where actual values are assigned to all measurable quantities - including those which in quantum theory are associated with non-commuting Hermitian operators. The actual values are determined from the hidden variables, which are associated with a classical *probability distribution* (see for example Section 7.1 of [7]). The Bell inequalities involve the *mean value*  $E(A_i \times B_j)$  of the product of observables  $A_i$  and  $B_j$  for subsystems  $A, B$  respectively, for which there are two possible measured values,  $+1$  and  $-1$ . In hidden variable theory, the mean values  $E(A_i \times B_j)$  are given by

$$E(A_i \times B_j) = \int d\lambda P(\lambda) A_i(\lambda) B_j(\lambda) \quad (10)$$

where  $A_i(\lambda)$  and  $B_j(\lambda)$  are the values assigned to  $A_i$  and  $B_j$  when the hidden variable is  $\lambda$ , and  $P(\lambda)$  is the hidden variable probability distribution function. The possible values for  $A_i(\lambda)$  and  $B_j(\lambda)$  are  $+1$  and  $-1$ . The form given by Clauser et al [4] for *Bell's inequality* is  $|S| \leq 2$  where

$$S = E(A_1 \times B_1) + E(A_1 \times B_2) + E(A_2 \times B_1) - E(A_2 \times B_2) \quad (11)$$

The minus sign can actually be attached to any one of the four terms. A proof of the Bell inequalities may be found in [7], [8].

### 2.4.2 Non-Entangled State Result

It can be shown that the Bell inequalities *always* occur for non-entangled states (see Section 7.3 of the book by Vedral [7]). For Bell's inequalities we consider Hermitian operators  $\hat{A}_i$  and  $\hat{B}_j$  for subsystems  $A, B$  respectively, for which there are two eigenvalues  $+1$  and  $-1$ , where the operators are given by the components  $\hat{A}_i = a_i \cdot \hat{\sigma}_A$  and  $\hat{B}_j = b_j \cdot \hat{\sigma}_B$  of Pauli spin operators  $\hat{\sigma}_A$  and  $\hat{\sigma}_B$  along directions with unit vectors  $a_i$  and  $b_j$ . The corresponding quantum theory quantity for the Bell inequality is

$$S = E(\hat{A}_1 \otimes \hat{B}_1) + E(\hat{A}_1 \otimes \hat{B}_2) + E(\hat{A}_2 \otimes \hat{B}_1) - E(\hat{A}_2 \otimes \hat{B}_2) \quad (12)$$

where in quantum theory the mean value is given by  $E(\hat{A}_i \otimes \hat{B}_j) = \langle \hat{A}_i \otimes \hat{B}_j \rangle = \text{Tr}(\hat{\rho} \hat{A}_i \otimes \hat{B}_j)$ . For the general bipartite non-entangled state given by 1 it is easy to show that

$$S = \sum_R P_R \left( \langle \hat{A}_1 \rangle_R^A \langle \hat{B}_1 + \hat{B}_2 \rangle_R^B + \langle \hat{A}_2 \rangle_R^A \langle \hat{B}_1 - \hat{B}_2 \rangle_R^B \right) \quad (13)$$

where  $\langle \hat{A}_i \rangle_R^A = \text{Tr}(\hat{A}_i \hat{\rho}_R^A)$  and  $\langle \hat{B}_j \rangle_R^B = \text{Tr}(\hat{B}_j \hat{\rho}_R^B)$  are the expectation values of  $\hat{A}_i$  and  $\hat{B}_j$  for the sub-systems  $A, B$  in states  $\hat{\rho}_R^A$  and  $\hat{\rho}_R^B$  respectively. Now  $\langle \hat{A}_i \rangle_R^A$  and  $\langle \hat{B}_j \rangle_R^B$  must lie in the range  $-1$  to  $+1$ , so that  $\langle \hat{B}_1 \pm \hat{B}_2 \rangle_R^B$  must each lie in the range  $-2$  to  $+2$ . Hence

$$\begin{aligned} |S| &\leq \sum_R P_R \left( |\langle \hat{A}_1 \rangle_R^A| |\langle \hat{B}_1 + \hat{B}_2 \rangle_R^B| + |\langle \hat{A}_2 \rangle_R^A| |\langle \hat{B}_1 - \hat{B}_2 \rangle_R^B| \right) \\ &\leq \sum_R P_R \left( |\langle \hat{B}_1 + \hat{B}_2 \rangle_R^B| + |\langle \hat{B}_1 - \hat{B}_2 \rangle_R^B| \right) \\ &\leq 2 \end{aligned} \tag{14}$$

since to obtain  $|\langle \hat{B}_1 + \hat{B}_2 \rangle_R^B| = 2$  requires  $\langle \hat{B}_1 \rangle_R^B = \langle \hat{B}_2 \rangle_R^B = \pm 1$  and then  $|\langle \hat{B}_1 - \hat{B}_2 \rangle_R^B| = |\langle \hat{B}_1 \rangle_R^B - \langle \hat{B}_2 \rangle_R^B| = 0$ , or to obtain  $|\langle \hat{B}_1 - \hat{B}_2 \rangle_R^B| = 2$  requires  $\langle \hat{B}_1 \rangle_R^B = -\langle \hat{B}_2 \rangle_R^B = \pm 1$  and then  $|\langle \hat{B}_1 + \hat{B}_2 \rangle_R^B| = |\langle \hat{B}_1 \rangle_R^B + \langle \hat{B}_2 \rangle_R^B| = 0$ .

### 2.4.3 Bell Inequality Violation and Entanglement

It follows that for a general two mode non-entangled state  $|S|$  cannot violate the Bell inequality limit of 2. Thus, the violation of Bell inequalities proves that the quantum state must be entangled for the sub-systems involved, so Bell inequality violations are a test of entanglement. For entangled states such as the Bell state  $|\Psi_-\rangle$  (see [8], Section 2.5) the Bell inequality can be violated for the choice where  $a_1, a_2$  and  $b_1, b_2$  are orthogonal and  $a_1, a_2$  are parallel to  $b_1 - b_2, b_1 + b_2$  respectively (see [8], Section 5.1). Furthermore, an entangled quantum state and measurements on it cannot be described via a hidden variable theory - which caused Einstein to consider that quantum theory violated *realism*. Violation of Bell inequalities is clearly a *non-classical* feature, since classical physics envisages all physical quantities such as  $A_i$  and  $B_j$  having well-defined values, even if they are not known and have to be described via a probability distribution  $P(\lambda)$  of hidden quantities  $\lambda$  which determine their values.

## 2.5 Non-local Correlations

Another feature of entangled states is that they are associated with *strong correlations* for *observables* associated with *localised sub-systems* that are *well-separated*, a particular example being *EPR correlations* between non-commuting observables. Entangled states can exhibit this particular *non-classical* feature, which again cannot be accounted for via a hidden variable theory.



### 2.5.1 Hidden Variable Theory

Consider two operators  $\hat{\Omega}_A$  and  $\hat{\Omega}_B$  associated with sub-systems  $A$  and  $B$ . These would be Hermitian if observables are involved, but for generality this is not required. In a hidden variable theory these would be associated with functions  $\Omega_C(\lambda)$  ( $C = A, B$ ) of the hidden variable  $\lambda$ , with the Hermitean adjoints  $\hat{\Omega}_C^\dagger$  being associated with the complex conjugates  $\Omega_C^*(\lambda)$ . *Correlation functions* given by the following mean values

$$\begin{aligned} E(\Omega_A^* \times \Omega_B) &= \int d\lambda P(\lambda) \Omega_A^*(\lambda) \Omega_B(\lambda) \\ E(\Omega_A^* \Omega_A \times \Omega_B^* \Omega_B) &= \int d\lambda P(\lambda) \Omega_A^*(\lambda) \Omega_A(\lambda) \Omega_B^*(\lambda) \Omega_B(\lambda) \end{aligned} \quad (15)$$

satisfy the following *correlation inequality*

$$|E(\Omega_A^* \times \Omega_B)|^2 \leq E(\Omega_A^* \Omega_A \times \Omega_B^* \Omega_B) \quad (16)$$

This result is based on the inequality

$$\int d\lambda P(\lambda) C(\lambda) \geq \left( \int d\lambda P(\lambda) \sqrt{C(\lambda)} \right)^2 \quad (17)$$

for real, positive functions  $C(\lambda), P(\lambda)$  and where  $\int d\lambda P(\lambda) = 1$ , and which is proved in Appendix 9. In the present case we have  $C(\lambda) = \Omega_A^*(\lambda) \Omega_A(\lambda) \Omega_B^*(\lambda) \Omega_B(\lambda)$ , which is real, positive. A violation of the inequality in Eq. (16) is an indication of strong correlation between sub-systems  $A$  and  $B$ .

### 2.5.2 Non-Entangled State Result

It can be shown that the correlation inequalities are *always* satisfied for non-entangled states. In quantum theory the correlation functions are given by  $E(\hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B) = \langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle = \text{Tr}(\hat{\rho} \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B)$  and  $E(\hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B) = \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle = \text{Tr}(\hat{\rho} \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B)$ . For a non-entangled state of sub-systems  $A$  and  $B$  we have

$$\begin{aligned} E(\hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B) &= \sum_R P_R \langle \hat{\Omega}_A^\dagger \rangle_R^A \langle \hat{\Omega}_B \rangle_R^B \\ E(\hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B) &= \sum_R P_R \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B \end{aligned} \quad (18)$$

Now

$$|E(\hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B)| \leq \sum_R P_R |\langle \hat{\Omega}_A^\dagger \rangle_R^A| |\langle \hat{\Omega}_B \rangle_R^B| \quad (19)$$

since the modulus of a sum is always less than the sum of the moduli. Using  $\langle (\hat{\Omega}_C^\dagger - \langle \hat{\Omega}_C^\dagger \rangle) (\hat{\Omega}_C - \langle \hat{\Omega}_C \rangle) \rangle \geq 0$  with  $(C = A, B)$ , we obtain the Schwarz

inequality - which is true for all states -  $\langle \hat{\Omega}_C^\dagger \hat{\Omega}_C \rangle \geq \langle \hat{\Omega}_C^\dagger \rangle \langle \hat{\Omega}_C \rangle = |\langle \hat{\Omega}_C \rangle|^2 = |\langle \hat{\Omega}_C^\dagger \rangle|^2$ , and hence

$$|E(\hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B)| \leq \sum_R P_R \sqrt{\langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A} \sqrt{\langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B} \quad (20)$$

Next we use the inequality

$$\sum_R P_R C_R \geq \left( \sum_R P_R \sqrt{C_R} \right)^2 \quad (21)$$

for real, positive functions  $C_R, P_R$  and where  $\sum_R P_R = 1$ . This inequality, which was used in the paper by Hillery et al [29], is proved in Appendix 9. In the present case we have  $C_R = \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B$  so that

$$|E(\hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B)|^2 \leq \sum_R P_R \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \rangle_R^A \langle \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle_R^B = E(\hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B) \quad (22)$$

Thus for a *non-entangled state* we obtain the *correlation inequality*

$$|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 = |\langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle|^2 \leq \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle \quad (23)$$

where the general result  $\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle = \langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle^*$  has been used. Thus non-entangled states have correlation functions that are consistent with hidden variable theory.

### 2.5.3 Weak Correlation Violation and Entanglement

Hence if it is found that the correlation inequality is violated  $|\langle \hat{\Omega}_A^\dagger \otimes \hat{\Omega}_B \rangle|^2 = |\langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle|^2 > \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle$  then the state must be entangled, so the correlation inequality violation is also a test for entanglement. Again entangled states have features that cannot be explained via hidden variable theory, so entangled states are clearly non-classical. ..

## 2.6 Identical Particles - Symmetrisation Principle

### 2.6.1 Symmetrization and Second Quantization

Whether *entangled* or *not* the physical states for systems of *identical particles* must conform to the *symmetrisation principle*, whereby the overall density operator has to be invariant under *permutation operators*. Problems arise regarding how to define non-entangled states for systems of identical particles. The basic

issue is how first to distinguish what are meaningful *sub-systems* for identical particle systems. Some authors ([41], [49].. ) consider states of the form

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes \dots \quad (24)$$

to be non-entangled states, where  $\hat{\rho}_R^i$  is a density operator for particle  $i$ . However such a state would not in general be physical, since the symmetrisation principle would be violated unless the  $\hat{\rho}_R^i$  were related. For example, consider the state for two identical bosonic atoms given by

$$\hat{\rho} = P_{\sigma\xi} \hat{\sigma}^1 \otimes \hat{\xi}^2 + P_{\theta\eta} \hat{\theta}^1 \otimes \hat{\eta}^2 \quad (25)$$

and apply the permutation  $\hat{P} = \hat{P}(1 \leftrightarrow 2)$ . The invariance of  $\hat{\rho}$  in general requires  $\hat{\sigma} = \hat{\xi}$  and  $\hat{\theta} = \hat{\eta}$ , giving  $\hat{\rho} = P_{\sigma} \hat{\sigma}^1 \otimes \hat{\sigma}^2 + P_{\theta} \hat{\theta}^1 \otimes \hat{\theta}^2$ . This is a statistical mixture of two states, one with both atoms in state  $\hat{\sigma}$ , the other with atoms in state  $\hat{\theta}$ . Of course if the atoms were all different (atom 1 a  $\text{Rb}^{87}$  atom, atom 2 a  $\text{Na}^{23}$  atom, ..) then the expression (25) would be a valid non-entangled state, but there the atomic sub-systems are distinguishable and symmetrisation is not required. What is distinguishable for systems of identical bosons is not the individual particles themselves - which do not carry labels, boson 1, boson 2, etc. - but the *single particle states* or *modes* that the bosons may occupy. For bosonic atoms with several hyperfine components, each component will have its own set of modes. The same would apply to fermionic atoms. For photons the modes may be specified via wave vectors and polarisations. Although the quantum pure states can be specified via symmetrized products of single particle states occupied by specific particles using a *first quantization* approach, it is more convenient to use *second quantization*. Here, a basis set for the quantum states of such sub-systems are the *Fock states*  $|n_a\rangle$  ( $n_a = 0, 1, 2, \dots$ ) etc, which specify the number of identical particles occupying the mode  $A$ , etc., so in this approach the mode is the sub-system and the Fock states give different physical states for this sub-system. Symmetrization is built into the definition of the Fock states. If the atoms were fermions rather than bosons the Pauli exclusion principle would of course restrict  $n_a = 0, 1$  only. Thus in this second quantization approach situations with differing numbers of identical particles are different *states*, not different *systems*. The overall system will be associated with physical states with density operators and state vectors in Fock space, which includes states with total numbers of identical particles ranging from zero in the vacuum state right up to infinity.

## 2.6.2 Sub-Systems and Modes

The point of view in which the possible *sub-systems*  $A$ ,  $B$ , etc are *modes* (or *sets* of modes) rather than *particles* has been adopted by several authors ([11], [12], [13]), [7], [21], [22] and will be the approach used here. What are or are not entangled are *modes* not *particles*. Overall, the system is a collection

of modes, not particles. Particles are associated with mode occupancies, and therefore related to specifying the quantum states of the system, rather than the system itself. Note that in this approach states where there is only a *single atom* may still be entangled states - for example with two spatial modes  $A, B$  the states which are a quantum superposition of the atom in each of these modes, such as the Bell state  $(|1_a\rangle|0_b\rangle + |0_a\rangle|1_b\rangle)/\sqrt{2}$  are entangled states. For entangled states associated with the EPR paradox or for quantum teleportation, the mode functions may be *localised* in well-separated spatial regions - spooky action at a distance - but spatially overlapping mode functions apply in other situations. Furthermore, as well as being distinguishable the modes can act as *separate systems*, with other modes being ignored. For interacting bosonic atoms this is much harder to accomplish experimentally than for the case of photons, where the relatively slow processes in which photons are destroyed in one EM field mode and created in another may require the presence of atoms as intermediaries. Two bosonic atoms in one mode may collide rapidly disappear into other modes. However, atomic boson interactions can be made very small via *Feshbach resonance* methods. Near absolute zero the basic physics of a BEC in a single trap potential is describable via a *one mode theory*. Hence with  $A, B, ..$  signifying distinct modes, the general non-entangled state is given in Eq. (1) though the present paper mainly involves only two modes.

Note however that a different concept of entanglement - *particle entanglement* - has also been applied to identical particle systems [19], [44]. This is not the same as mode entanglement so tests and measures for particle entanglement will differ from those for mode entanglement. For completeness a brief description highlighting the difference between mode and particle entanglement is presented in Appendix 10. A further discussion about the distinction is given in [18].

### 2.6.3 Multi-Mode Sub-Systems

As well as the simple case where the sub-systems are all *individual* modes, the concept of entanglement may be *extended* to situations where the sub-systems are *sets of modes*, rather than individual modes. In this case entanglement or non-entanglement will be of these distinct sets of modes. Such a case is considered in Subsection 5.3, where *pairs* of modes associated with distinct lattice sites are considered as the sub-systems. Another example is treated in He et al [50], which involves a double well potential with each well associated with two bosonic modes, these pairs of modes being the two sub-systems. Entanglement criteria for the mode pairs based on local spin operators associated with each potential well are considered (see SubSection 5.6). A further example is treated by Heaney et al [51], again involving four modes associated with a double well potential. As in the previous example, each mode pair is associated with the same well in the potential, but here a Bell entanglement test was obtained for pairs of modes in the different wells. The concept of *entanglement of sets of modes* is a straightforward extension of the basic concept of entanglement of individual modes.

## 2.7 Super-Selection Rule

### 2.7.1 Global Particle Number SSR

The question of what physical states - entangled or not - are possible in the *non-relativistic quantum physics* of a system of identical *bosonic* particles - such as bosonic *atoms* or *photons* - has been the subject of much discussion. Whether *entangled* or *not* it is generally accepted that there is a *super-selection rule* that prohibits *quantum superposition states* of the form

$$|\Phi\rangle = \sum_{N=0}^{\infty} C_N |N\rangle \quad \hat{\rho} = \sum_{N=0}^{\infty} |C_N|^2 |N\rangle \langle N| + \sum_{N=0}^{\infty} \sum_{M=0}^{\infty} (1 - \delta_{N,M}) C_N C_M^* |N\rangle \langle M| \quad (26)$$

being *physical* states when they involve Fock states  $|N\rangle$  with differing total numbers  $N$  of particles. The density operator for such a state would involve *coherences* between states with differing  $N$ . Although such superpositions - such as the *Glauber coherent state*  $|\alpha\rangle$ , where  $C_N = \exp(-|\alpha|^2/2) \alpha^N / \sqrt{N!}$  - do have a useful *mathematical* role, they do *not* represent actual physical states according to the super-selection rule. The papers by Sanders et al [36] and Cable et al [52] are examples of applying the SSR for optical fields, but also using the mathematical features of coherent states to treat phenomena such as interference between independent lasers. The super-selection rule indicates that the most *general physical state* for a system of identical bosonic particles can only be of the form

$$\begin{aligned} \hat{\rho} &= \sum_{N=0}^{\infty} \sum_{\Phi} P_{\Phi N} (|\Phi_N\rangle \langle \Phi_N|) \\ |\Phi_N\rangle &= \sum_i C_i^N |N i\rangle \end{aligned} \quad (27)$$

where  $|\Phi_N\rangle$  is a quantum superposition of states  $|N i\rangle$  each of which involves exactly  $N$  particles, and where different states with the same  $N$  are designated as  $|N i\rangle$ . This state  $\hat{\rho}$  is a statistical mixture of states, each of which contains a specific number of particles. Such a SSR is referred to as a *global* SSR, as it applies to the system as a whole. Mathematically, the global particle number SSR can be expressed as

$$[\hat{N}, \hat{\rho}] = 0 \quad (28)$$

where  $\hat{N}$  is the *total number* operator.

### 2.7.2 Examples of Global Particle Number SSR Compliant States

Examples of a state vector  $|\Phi_N\rangle$  for an entangled pure state [12] and a density operator  $\hat{\rho}$  for a non-entangled mixed [53] state for a two mode bosonic system, both of which are possible physical states are

$$|\Phi_N\rangle = \sum_{k=0}^N C(N, k) |k\rangle_A \otimes |N - k\rangle_B \quad (29)$$

$$\hat{\rho} = \sum_{k=0}^N P(k) |k\rangle_A \langle k|_A \otimes |N - k\rangle_B \langle N - k|_B \quad (30)$$

The entangled pure state is a superposition of product states with  $k$  bosons in mode  $A$  and the remaining  $N - k$  bosons in mode  $B$ . Every term in the superposition is associated with the same total boson number  $N$ . The non-entangled mixed state is a statistical mixture of product states also with  $k$  bosons in mode  $A$  and the remaining  $N - k$  bosons in mode  $B$ . Every term in the statistical mixture is associated with the same total boson number  $N$ . For the case of a two mode fermionic system the Pauli exclusion principle restricts the number of possible fermions to two, with at most one fermion in each mode. Expressions for a state with exactly  $N = 2$  fermions are

$$|\Phi_2\rangle = |1\rangle_A \otimes |1\rangle_B \quad (31)$$

$$\hat{\rho} = |1\rangle_A \langle 1|_A \otimes |1\rangle_B \langle 1|_B \quad (32)$$

Neither state is entangled and both are the same pure state since  $\hat{\rho} = |\Phi_2\rangle \langle \Phi_2|$ . Although the super-selection rules and symmetrisation principle also applies to fermions, as indicated in the Introduction this paper is focused on bosonic systems, and it will be assumed that the modes are bosonic unless indicated otherwise.

The Bell states for  $N = 2$  bosons provide important examples of four mode pure quantum states that are compliant with the global particle number SSR. The modes are designated  $A+, A-, B+, B-$  and the Fock states are in general  $|n_{A+}, n_{A-}, n_{B+}, n_{B-}\rangle$ . The Bell states may be written

$$\begin{aligned} |\Psi_{\text{singlet}}\rangle &= \frac{1}{\sqrt{2}}(|1, 0, 0, 1\rangle - |0, 1, 1, 0\rangle) \equiv \frac{1}{\sqrt{2}}(|A+\rangle \otimes |B-\rangle - |A-\rangle \otimes |B+\rangle) \\ |\Psi_{\text{triplet},+1}\rangle &= |1, 0, 1, 0\rangle \equiv |A+\rangle \otimes |B+\rangle \\ |\Psi_{\text{triplet},0}\rangle &= \frac{1}{\sqrt{2}}(|1, 0, 0, 1\rangle + |0, 1, 1, 0\rangle) \equiv \frac{1}{\sqrt{2}}(|A+\rangle \otimes |B-\rangle + |A-\rangle \otimes |B+\rangle) \\ |\Psi_{\text{triplet},-1}\rangle &= |0, 1, 0, 1\rangle \equiv |A-\rangle \otimes |B-\rangle \end{aligned} \quad (33)$$

where the second forms may be more familiar. Of these states  $|\Psi_{\text{singlet}}\rangle$  and  $|\Psi_{\text{triplet},0}\rangle$  are entangled, whilst  $|\Psi_{\text{triplet},+1}\rangle$  and  $|\Psi_{\text{triplet},-1}\rangle$  are separable.

### 2.7.3 Super-Selection Rules and Conservation Laws

It is important to realise that such super-selection rules are *additional constraints* to those imposed by *conservation laws*. For example, the conservation law on total particle number *only* leads to the requirement on the superposition state  $|\Phi\rangle$  that the  $|C_N|^2$  are time independent, it does *not* require only one  $C_N$  being non-zero. Super-selection rules are broad in their scope, forbidding quantum superpositions of states of systems with differing charge, differing baryon number and differing statistics. Thus a combined system of a hydrogen atom and a helium ion does not exist in quantum states that are linear combinations of hydrogen atom states and helium ion states - the super-selection rules on both charge and baryon number preclude such states. The basis physical states for such a combined system would involve symmetrised tensor products

of hydrogen atom and helium ion states, not linear combinations - symmetrisation being required because the system contains two identical electrons. On the other hand, super-selection rules do not prohibit quantum superpositions of states of systems with differing energy, angular or linear momenta - other physical quantities that may also be conserved. Thus in a hydrogen atom quantum superpositions of states with differing energy and angular momentum quantum numbers are allowed physical states.

#### 2.7.4 SSR Justification and No Suitable Phase Reference

There are two types of justification for applying the super-selection rules for systems of identical particles. The first approach is based on simple considerations and will be outlined below in this subsection. The second approach [34], [35], [36], [37], [38], [39], [26], [31], [32], [16] is more sophisticated and involves linking the absence or presence of SSR to whether or not there is a suitable *reference frame* in terms of which the quantum state is described, and is outlined in the next subsection and Appendix 11. The key idea is that SSR are a consequence of considering the description of a quantum state by an external observer (Charlie) whose phase reference frame has an unknown phase difference from that of an observer ((Alice) more closely linked to the system being studied. Thus, whilst Alice's description of the quantum state may violate the SSR, the description of the *same* quantum state by Charlie will not. In the main part of this paper the density operator  $\hat{\rho}$  used to describe the various quantum states will be that of the external observer (Charlie).

#### 2.7.5 SSR Justification and Physics Considerations

A number of *straightforward reasons* have been given in the Introduction for why it is appropriate to apply the superselection rule to exclude quantum superposition states of the form (26) as physical states for systems of identical particles, and these will now be considered in more detail.

Firstly, no way is known for creating such states. The Hamiltonian for such a system commutes with the total boson number operator, resulting in the  $|C_N|^2$  remaining constant, so the quantum superposition state would need to have existed initially. In the simplest case of non-interacting bosonic atoms, the Fock states are also energy eigenstates, such Fock states involve total energies that differ by energies of order the rest mass energy  $mc^2$ , so a coherent superposition of states with such widely differing energies would at least seem unlikely in a *non-relativistic theory*, though for massless photons this would not be an issue as the energy differences are of order the photon energy  $\hbar\omega$ . The more important question is: Is there a non-relativistic quantum process could lead to the creation of such a state? Processes such as the dissociation of  $M$  diatomic molecules into up to  $2M$  bosonic atoms under Hamiltonian evolution involve entangled atom-molecule states of the form

$$|\Phi\rangle = \sum_{m=0}^M C_m |M-m\rangle_{mol} \otimes |2m\rangle_{atom} \quad (34)$$

but the reduced density operator for the bosonic atoms is

$$\hat{\rho}_{atoms} = \sum_{m=0}^M |C_m|^2 (|2m\rangle \langle 2m|)_{atom} \quad (35)$$

which is a statistical mixture of states with differing atom numbers with no coherence terms between such states. Such statistical mixtures are valid physical states, corresponding to a lack of a priori knowledge of how many atoms have been produced. To obtain a quantum superposition state for the atoms *alone*, the atom-molecule state vector would need to evolve at some time into the form

$$|\Phi\rangle = \sum_{m=0}^M B_m |M-m\rangle_{mol} \otimes \sum_{n=0}^M A_{2n} |2n\rangle_{atom} \quad (36)$$

where the separate atomic system is in the required quantum superposition state. However if such a state existed there would be terms with at least one non-zero coefficient  $B_m A_{2n}$  involving product states  $|M-m\rangle_{mol} \otimes |2n\rangle_{atom}$  with  $n \neq m$  if the state  $|\Phi\rangle$  is not just in the entangled form (34). However, the presence of such a term would mean that the conservation law involving the number of molecules plus two times the number of atoms was violated. This is impossible, so such an evolution is not allowed.

Secondly, no way is known for measuring all the properties of such states, even if they existed. If a state such as (26) did exist then the amplitudes  $C_N$  would oscillate with frequencies that differ by relativistic frequencies of order  $mc^2/\hbar$ , even if boson-boson interactions were included. To distinguish the phases of the  $C_N$  in order to verify the existence of the state, *measurement operators* would need to include terms that also oscillate at relativistic frequencies, and no such measurement operators are known.

Thirdly, there is no need to invoke the existence of such states in order to understand coherence and interference effects. It is sometimes thought that states involving quantum superpositions of number states are needed for discussing *coherence* and *interference properties* of BECs, and some papers describe the state via the Glauber coherent states. However, as Leggett [54] has pointed out (see also Bach et al [55], Dalton and Ghanbari [56]), a highly occupied number state for a single mode with  $N$  bosons has coherence properties of high order  $n$ , as long as  $n \ll N$ . The introduction of a Glauber coherent state is *not* required to account for coherence effects. Even the well-known presence of spatial interference patterns produced when two independent BECs are overlapped can be accounted for via treating the BECs as Fock states. The interference pattern is built up as a result of successive boson position measurements [57], [36], [52].

Fourthly, the stability of such states against decoherence processes may not be great, so even if they could be created, they could rapidly change to other states. However, decoherence time scales that are not too short would be acceptable. Although BECs are created in high vacuum experiments and are well isolated from the external environment in magnetic or dipole traps, they are not entirely free from decoherence effects because the bosons do interact with each other. Even in a single mode case boson-boson collisions can cause dephasing



effects. These could be shown via the decay of the coherence  $\langle \hat{a} \rangle$ . However, it may turn out that the lifetime of a coherent state in a single mode BEC is quite long - in the case of photons the lifetime could be as long as the inverse Townes-Schawlow line width, perhaps of order  $10^3$ s (see below). If a coherent superposition state could be created with a non-zero coherence, this may last long enough to carry out further experiments, so this fourth reason for discarding coherent superposition states is relatively unimportant though further studies of their lifetimes would be of some theoretical interest. .

### 2.7.6 SSR Justification and Galilean Frames ?

Finally, in addition to the previous reasons there is an argument based on the requirement that the dynamical equations for such non-relativistic quantum systems should be invariant under a *Galilean transformation* which has been proposed [58] as a proof of the super-selection rule for atom number. This approach is linked to the reference frame based justification of SSR (see Appendix 11). However, whilst the paper shows that under a Galilean transformation - corresponding to describing the system from the point of view of an observer moving with a constant velocity  $\mathbf{v}$  with respect to the original observer, and where the two observers have identical clocks - the terms in a superposition state with different numbers  $N$  of massive bosons would oscillate like  $\exp i (\frac{1}{2} N m \mathbf{v}^2 t) / \hbar$ , such oscillations have non-relativistic frequency differences, and are only to be expected if the *same* quantum state is described by a moving observer. This feature alone does not seem to require the super-selection rule, since here the moving observer's reference frame has a well-defined velocity with respect to that attached to the system so that no twirling operation resulting in the elimination of number state coherences is involved (see Appendix 11), and so will not be considered further in this paper.

On the other hand, an approach of this kind involving *rotation symmetry* would seem to rule out such states as quantum superpositions of a boson (spin 0) and a fermion (spin 1/2). Let such a state be prepared in the form  $(|F\rangle + |B\rangle)/\sqrt{2}$ . Consider an observer whose cartesian reference frame is  $X, Y, Z$ . This is a classical system that can be rotated in space. If the observer rotates with his frame through  $2\pi$  about any axis they are then back in the same position, but the observer now sees the state as  $(-|F\rangle + |B\rangle)/\sqrt{2}$ . This state is apparently orthogonal to the one observed before the rotation, and this is paradoxical since the observer would be in the same position. Thus there is a super-selection rule excluding states such as  $(|F\rangle + |B\rangle)/\sqrt{2}$ . A similar argument based on the *time reversal* anti-unitary operator was given by Wick et al [24].

### 2.7.7 SSR and Photons

Though this paper is focused on massive bosonic atoms similar considerations also apply to the optical quantum EM field, which involve *massless* bosons - *photons*. Even in the case of photons, Molmer [59] has argued that the physical state for a single mode optical laser field operating well above threshold is not a

Glauber coherent state, and the density operator would be a statistical mixture of the form (27), with  $|\Phi_N\rangle = |N\rangle$  and  $P_{\Phi_N} = \exp(-\bar{N}) \bar{N}^N / N!$ . Here the density operator is a statistical mixture of photon number states with Poisson distribution, or equivalently a statistical mixture of coherent states  $|\alpha\rangle$  with  $\alpha = \sqrt{\bar{N}} \exp(i\phi)$  and all phases  $\phi$  having equal probability. The same general reasons for applying the super-selection rule to systems of identical massive bosons also apply here, though the details differ. For the free quantum EM field there is a conservation law for the photon number in each mode, so in this case again  $|C_N|^2$  would be time independent. Here the  $C_N$  would oscillate with frequencies that only differ by non-relativistic frequencies of order  $\hbar\omega$ , so the argument against coherent states based on this feature do not apply. However, in the case of the single mode optical laser, the field is generated via interactions with incoherently pumped atoms, there is no well defined optical phase that can be imposed on the process and the quantum theory for such laser processes predicts a quantum state that is a statistical mixture of photon number states. In the case of the optical laser field coherent states are not physical because there are no optical reference fields with a well-defined phase that could be used to determine the phases associated with the expansion coefficients. Optical interference and coherence effects can also be explained without invoking Glauber coherent states, as [59] and others such as [36] have shown. However, if coherent states could be created they might be relatively stable. In the optical laser field case, phase loss via diffusion is related to the laser linewidth, and this can be reduced to the Townes-Schawlow limit that varies inversely as the mean photon number - which is large. The Townes-Schawlow linewidth can be as small as  $10^{-3}$  hz, corresponding to a phase diffusion time of  $10^3$  s. An alternative approach is presented by Wiseman et al [60], [61], in which the optical laser is treated via a master equation, but where monitoring of the laser environment (difficult!) is required to determine whether certain pure state ensembles - such as those involving coherent states - are physically realisable. The conclusion reached is that for finite self energy the coherent state ensemble is not physically realisable, the closest ensemble being that involving squeezed states, though for zero self energy coherent state ensembles are obtained.

There is however, an approach (see next sub-section and SubSection 11.4 in Appendix 11) involving the consideration of phase reference frames, in terms of which the quantum state of a single mode laser may be described as a Glauber coherent state by an observer (Alice) with one reference frame, but would be described as a statistical mixture of photon number states by another observer (Charlie) with a different reference frame, whose phase reference is completely unrelated to the previous one.

## 2.8 Reference Frames and Violations of Superselection Rules

Challenges to the requirement for physical states to be consistent with super-selection rules have occurred since the 1960's when Aharonov and Susskind [34] suggested that coherent superpositions of different charge eigenstates could be

created. It is argued that super-selection rules are not a fundamental requirement of quantum theory, but the restrictions involved could be lifted if there is a suitable system that acts as a *reference* for the coherences involved - [34], [35], [36], [37], [38], [39], [26], [31], [32], [16] provide discussions regarding reference systems and SSR.

### 2.8.1 Linking SSR and Reference Frames

The discussion of the super-selection rule issue in terms of reference systems is quite complex and too lengthy to be covered in the body of this paper. However, in view of the wide use of the reference frame approach a full outline is presented in Appendix 11. The key idea is that there are two observers - Alice and Charlie - who are describing the same quantum state in terms of their own reference systems. The reference systems are *macroscopic systems* in states where the behaviour is essentially *classical*, such as large magnets that can be used to define *cartesian axes* or BEC in Glauber coherent states that are introduced to define a *phase reference*. The relationship between the two reference systems is represented by a *group* of *unitary transformation operators* listed as  $\hat{T}(g)$ , where the particular transformation (translation or rotation of cartesian axes, phase change of phase references, ..) that changes Alice's reference system into Charlie's is denoted by  $g$ . Alice is the *internal* observer, closely linked to the system under study and describes the quantum state via her density operator, whereas Charlie is the *external* observer whose specification of the *same* quantum state via his density operator is of most interest. There are two cases of importance, *Situation A* - where the relationship between Alice's and Charlie's reference frame is *known* and specified by a *single* parameter  $g$ , and *Situation B* - where on the other hand the relationship between frames is completely *unknown*, all possible transformations  $g$  must be given equal weight. Situation A is not associated with SSR, whereas Situation B leads to SSR. The relationship between Alice's and Charlie's density operators is given in terms of the transformation operators (see Eq. (199) for Situation A and Eq. (200) for Situation B). In Situation B there is often a qualitative change between Alice's and Charlie's description of the same quantum state, with pure states as described by Alice becoming mixed states when described by Charlie. It is Situation B with the  $U(1)$  transformation group - for which *number operators* are the *generators* - that is of interest for the *single* or *multi-mode* systems involving *identical bosons* on which the present paper focuses. An example of the qualitative change of behaviour for the single mode case is that *if* it is *assumed* that Alice could prepare the system in a Glauber coherent pure state - which involves SSR breaking coherences between differing number states - then Charlie would describe the same state as a Poisson statistical mixture of number states - which is consistent with the operation of the SSR. Thus the SSR applies in terms of external observer Charlie's description of the state. This is how the dispute on whether the state for single mode laser is a coherent state or a statistical mixture is resolved - the two descriptions apply to different observers - Alice and Charlie. On the other hand there are quantum states such as Fock states

and Bell states which are described the same way by both Alice and Charlie, even in Situation B. The general justification of the SSR for Charlie's density operator description of the quantum state in Situation B is derived in terms of the *irreducible representations* of the transformation group, there being no coherences between states associated with differing irreducible representations (see Eq. (224)). For the particular case of the  $U(1)$  transformation group the irreducible representations are associated with the total *boson number* for the system or sub-system, hence the SSR that prohibits coherences between states where this number differs. Finally, it is seen that if Alice describes a general non-entangled state of sub-systems - which being separable have their own reference frames - then Charlie will also describe the state as a non-entangled state and with the same probability for each product state (see Eqs. (229) and (230)). For systems involving *identical bosons* Charlie's description of the sub-system density operators will only involve density operators that conform to the SSR. This is in accord with the key idea of the present paper.

### 2.8.2 Coherent Superposition of Atom and Molecule ?

Based around the reference frame approach Dowling et al [62] and Terra Cunha et al [13] propose processes using a BEC as a reference system that would create a coherent superposition of an atom and a molecule, or a boson and a fermion [62]. Dunningham et al [63] consider a scheme for observing a superposition of a one boson state and the vacuum state. Obviously if super-selection rules can be overcome in these instances, it might be possible to *produce* coherent superpositions of Fock states with differing particle numbers such as Glauber coherent states, though states with  $\overline{N} \sim 10^8$  would presumably be difficult to produce. However, detailed considerations of such papers indicate that the states actually produced in terms of Charlie's description are statistical mixtures consistent with the super-selection rules rather than coherent superpositions, which are only present in Alice's description of the state. Also, although coherence and interference effects are demonstrated, these can also be accounted for without invoking the presence of coherent superpositions that violate the super-selection rule. As the paper by Dowling et al [62] entitled "Observing a coherent superposition of an atom and a molecule." is a good example of where the super-selection rules are challenged, the key points are described in Appendix 12. Essentially the process involves one atom  $A$  interacting with a BEC of different atoms  $B$  leading to the creation of one molecule  $AB$ , with the BEC being depleted by one  $B$  atom. There are three stages in the process, the first being with the interaction that turns separate atoms  $A$  and  $B$  into the molecule  $AB$  turned on at Feshbach resonance for a time  $t$  related to the interaction strength and the mean number of bosons in the BEC reference system, the second being free evolution at large Feshbach detuning  $\Delta$  for a time  $\tau$  leading to a phase factor  $\phi = \Delta \tau$ , the third being again with the interaction turned on at Feshbach resonance for a further time  $t$ . However, it is pointed out in Appendix 12 that Charlie's description of the state produced for the atom plus molecule system is merely a statistical mixture of a state with one atom and no molecules and

a state with no atom and one molecule, the mixture coefficients depending on the phase  $\phi$  imparted during the process. However a coherent superposition is seen in Alice's description of the final state, though this is not surprising since a SSR violating initial state was assumed. The feature that in Charlie's description of the final state no coherent superposition of an atom and a molecule is produced in the process is not really surprising, because of the averaging over phase differences in going from Alice's reference frame to Charlie's. It is the dependence on the phase  $\phi$  imparted during the process that demonstrates coherence (Ramsey interferometry) effects, but it is shown in Appendix 12 that exactly the same results can be obtained via a treatment in which states which are coherent superpositions of an atom and a molecules are never present, the initial BEC state being chosen as a Fock state. In terms of the description by an external observer (Charlie) the claim of violating the super-selection rule has not been demonstrated via this particular process.

### 2.8.3 Detection of SSR Violating States

Whether such super-selection rule violating states can be *detected* has also not been justified. For example, consider the state given by a superposition of a one boson state and the vacuum state (as discussed in [63]). We consider an interferometric process in which one mode  $A$  for a two mode BEC interferometer is initially in the state  $\alpha|0\rangle + \beta|1\rangle$ , and the other mode  $B$  is initially in the state  $|0\rangle$  - thus  $|\Psi(i)\rangle = (\alpha|0\rangle + \beta|1\rangle)_A \otimes |0\rangle_B$  in the usual occupancy number notation, where  $|\alpha|^2 + |\beta|^2 = 1$ . The modes are first coupled by a beam splitter, then a free evolution stage occurs for time  $\tau$  associated with a phase difference  $\phi = \Delta\tau$  (where  $\Delta = \omega_B - \omega_A$  is the mode frequency difference), the modes are then coupled again by the beam splitter and the probability of an atom being found in modes  $A, B$  finally being measured. The probabilities of finding one atom in modes  $A, B$  respectively are found to only depend on  $|\beta|^2$  and  $\phi$ . Details are given in Appendix 12. There is no dependence on the relative phase between  $\alpha$  and  $\beta$ , as would be required if the superposition state  $\alpha|0\rangle + \beta|1\rangle$  is to be specified. Exactly the same detection probabilities are obtained if the initial state is the mixed state  $\hat{\rho}(i) = |\alpha|^2(|0\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B) + |\beta|^2(|1\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B)$ , in which the vacuum state for mode  $A$  occurs with a probability  $|\alpha|^2$  and the one boson state for mode  $A$  occurs with a probability  $|\beta|^2$ . In this example the proposed coherent superposition associated with the super-selection rule violating state would not be detected in this interferometric process, nor in the more elaborate scheme discussed in [63].

## 2.9 Super-Selection Rule - Separate Sub-Systems

### 2.9.1 Local Particle Number SSR

We now consider the role of the super-selection rule for the case of *non-entangled* states. The global super-selection rule on *total particle number* has restricted the physical quantum state for a system of identical bosons to be of the form

(27). Such states may or may not be entangled states of the modes involved. The question is - do similar restrictions involving the *sub-system particle number* apply to the modes, considered as *separate* sub-systems in the definition of non-entangled states ? The viewpoint in this paper is that this is so. Note that applying the SSR on the separate sub-system density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  is *only* in the context of non-entangled states. Such a SSR is referred to as a *local* SSR, as it applies to each of the separate sub-systems. Mathematically, the local particle number SSR can be expressed as

$$[\hat{N}_X, \hat{\rho}_R^X] = 0 \quad (37)$$

where  $\hat{N}_X$  is the *number* operator for sub-system  $X = A, B, \dots$ . The SSR restriction is based on the proposition that the density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  for the separate sub-systems  $A, B, \dots$  should themselves represent possible *physical states* for each of the sub-systems, considered as a *separate system* and thus be required to satisfy the super-selection rule that forbids quantum superpositions of Fock states with differing boson numbers. It is contended that expressions for the non-entangled quantum state  $\hat{\rho}$  in which  $\hat{\rho}_R^A, \hat{\rho}_R^B, \hat{\rho}_R^C, \dots$  were *not* physical states for the sub-systems would only be of mathematical interest.

Applying the local particle number SSR to the sub-system density operators for non-entangled states is discussed in papers by Bartlett et al [25], [26] as one of several *operational approaches* for defining entangled states. However, other authors such as [27], [28] state on the contrary that states when the sub-system density operators do *not* conform to the local particle number super-selection rule *are* still separable, others such as [29], [30] do so by implication, so in this paper we are advocating a *revision* to the *widely held notion* of entanglement in identical particle systems, the consequence being that the set of entangled states is now much *larger*. This is a *key idea* in this paper - not only should super-selection rules on particle numbers be applied to the *overall* physical state, entangled or not, but it *also* should be applied to the density operators that describe states of the modal *sub-systems* involved in the general definition of *non-entangled* states. The reasons for adopting this viewpoint are set out below. Apart from the papers by Bartlett et al [25], [26] we are not aware that this definition of non-entangled states has been invoked previously, indeed the opposite approach has been proposed [27], [28]. However, the idea of considering sub-system states which satisfy the local particle number SSR has been presented in several papers - [27], [28], [25], [26], [31], [32], [33], mainly in the context of pure states for bosonic systems, though in these papers the focus is on issues other than the definition of entanglement - such as quantum communication protocols [27], multicopy distillation [25], mechanical work and accessible entanglement [31], [32] and Bell inequality violation [33]. However, there are a number of papers that do not apply the SSR to the sub-system density operators, and those that do have not studied the consequences for various entanglement tests - as is done in the present paper.

### 2.9.2 Local SSR Justification and Independent Local Phase References

The more elaborate justification in terms of reference frames for this SSR requirement on non-entangled states is presented in SubSection 11.9 of Appendix 11. Essentially the idea is that in the context of separable states, each sub-system has its own *independent phase reference frames*, and those of Charlie having an unknown phase in relation to those of Alice. This leads to the local particle number SSR.

### 2.9.3 Local SSR Justification and Physics Considerations

The more simple reasons for this assertion are analogous to those for the overall multi-mode system and may be summarised as: absence of both a preparation process and a measurement process for such states, the lack of need of such states to describe single mode interference and coherence effects. Such superposition states may also be unstable, though again this is not a fatal problem.

Firstly, sub-system states incompatible with the SSR cannot be prepared. Consider for example a typical preparation process. For the situation of two modes  $A, B$  physically allowed pure states  $|\Phi_N\rangle$  could be prepared which in general are entangled states of the form

$$|\Phi_N\rangle = \sum_{k=0}^N A_k^N |k\rangle_A |N-k\rangle_B \quad (38)$$

so that the general mixed physical state for the two mode system is

$$\hat{\rho} = \sum_{N=0}^{\infty} \sum_{\Phi} P_{\Phi N} \sum_{k=0}^N \sum_{l=0}^N A_k^N (A_l^N)^* |k\rangle_A \langle l|_A \otimes |N-k\rangle_B \langle N-l|_B \quad (39)$$

Hence the reduced density operator - which specifies the state for mode  $A$  if measurements on this mode were carried out and measurements on other modes discarded - will be given by

$$\hat{\rho}_A = \sum_{N=0}^{\infty} \sum_{\Phi} P_{\Phi N} \sum_{k=0}^N A_k^N (A_k^N)^* |k\rangle_A \langle k|_A \quad (40)$$

which is a statistical mixture of Fock states  $|k\rangle_A$ . Thus the quantum state for mode  $A$  considered separately contains no superposition of states  $|k\rangle_A$  with differing numbers of bosons occupying mode  $A$ . As in the example considered in the previous section, the evolution of  $|\Phi_N\rangle$  into a tensor product of superposition states for modes  $A$  and  $B$  of the form

$$|\Phi_N\rangle = \sum_{k=0}^N C_k^N |k\rangle_A \otimes \sum_{k=0}^N D_k^N |N-k\rangle_B \quad (41)$$

is not possible. The preparation of the state for mode  $A$  must have involved first preparing a physical state for the full multi-mode system - for which the two

mode state in Eq. (39) is a specific example - from which the state associated with a particular mode is then determined as given by the reduced density operator. As illustrated by the example just given, the super-selection rule on the total number of identical bosons for the overall system produces a reduced density operator for the sub-system in which the super-selection rule for boson number also applies - that is the state for the sub-system does not involve quantum superpositions of mode Fock states with differing boson numbers, it only can involve statistical mixtures of such states.

Secondly, measurement processes may be applied to each separate mode and again the lack of measurement systems with well defined relativistic phases would preclude measurements that determine the rapidly varying phase differences between the expansion coefficients in single mode state vectors of the form  $|\Phi_A\rangle = \sum_{n=0}^{\infty} C_n |n\rangle_A$ . Invoking the existence of states whose key properties cannot be measured is somewhat dubious.

Thirdly, experimental setups involving single mode BECs and optical systems can be created and yet there is no need to invoke coherent superpositions of number states to explain coherence and interferometric effects. Thus essentially the *same reasons* that justify applying the super-selection rule to the overall many boson system also apply to the separate mode sub-systems.

#### 2.9.4 Local SSR Justification and Joint Measurements

A consideration of *joint measurements* on all the sub-systems leads to other fundamental reasons why the individual density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  in the specific situation of the general mixed non-entangled state given in Eq. (1) must represent physical states for the sub-systems. This state is a statistical mixture of product states  $\hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes \dots$  - each product state being an overall state of the system that *could* have been prepared. If sub-system  $A$  is prepared by one experimenter in state  $\hat{\rho}_R^A$  with probability  $P_R$ , classical communications to other local experimenters to prepare the other sub-systems in states  $\hat{\rho}_R^B, \hat{\rho}_R^C$ , etc with the same probability will result in the preparation of the overall mixed state. If such an overall product state is a physical state, then so must be the states of the uncorrelated sub-systems involved. Furthermore, measurements on *all* the sub-systems can be carried out, not just those on one particular sub-system  $A$  - where the results for the sub-system probabilities  $P_A(i)$  are determined from the reduced density operator  $\hat{\rho}_A$  - see Eq. (9). We have seen in Eq (4) that the joint probability  $P_{AB..}(i, j, \dots)$  for measurements on all the sub-systems is determined from the product of the individual sub-system probabilities  $P_A^R(i), P_B^R(j), \dots$  associated with sub-system density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$ , the overall product being weighted by the probability  $P_R$  that a particular product state is prepared. The reduced density operators for all the sub-systems do *not* determine this *joint probability* - what is required are the *full set* of sub-system density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  along with the overall probability  $P_R$  that a particular product state is prepared. As these individual sub-system probabilities  $P_A^R(i), P_B^R(j), \dots$  must determine actual possible measurements then the density



operators  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  must correspond to possible physical states for the sub-systems, the sub-systems being modes or single particle states in the present case. But as we have seen, the possible physical states that can be prepared for these sub-systems are those as in Eq. (40) which are a statistical mixture of number states with no coherences between Fock states with differing boson numbers, so the  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  themselves satisfy the super-selection rule.

### 2.9.5 Example of State that Violate Local and Global Particle Number SSR

Finally, an objection to applying the super-selection rule to separate modes based on emphasising only measurements on only one mode and its the reduced density operator may be raised, and suggest that  $\hat{\rho}_R^A, \hat{\rho}_R^B$  etc may be allowable provided that the overall reduced density operators comply with the super-selection rule. However, as will be seen this is not in general possible. As shown above, measurements on the subsystems with measurements on the other sub-systems discarded - are determined *only* from the reduced density operators  $\hat{\rho}_A = \sum_R P_R \hat{\rho}_R^A$  alone. Hence it may seem that providing the reduced density operators represent physical states then it does not matter if the  $\hat{\rho}_R^A, \hat{\rho}_R^B, \hat{\rho}_R^C, \dots$  do not. Indeed, for special cases we can find density operators  $\hat{\rho}_R^A$  that are unphysical even though the reduced density operator  $\hat{\rho}_A$  is physical. One such example is where

$$\begin{aligned}\hat{\rho}_1^A &= \left( \frac{1}{\sqrt{2}}(|0\rangle_A + |1\rangle_A) \right) \left( \frac{1}{\sqrt{2}}(\langle 0|_A + \langle 1|_A) \right) & P_1 &= \frac{1}{2} \\ \hat{\rho}_2^A &= \left( \frac{1}{\sqrt{2}}(|0\rangle_A - |1\rangle_A) \right) \left( \frac{1}{\sqrt{2}}(\langle 0|_A - \langle 1|_A) \right) & P_2 &= \frac{1}{2}\end{aligned}\quad (42)$$

which yields

$$\hat{\rho}_A = \frac{1}{2} (|0\rangle_A \langle 0|_A) + \frac{1}{2} (|1\rangle_A \langle 1|_A) \quad (43)$$

This is a valid statistical mixture of two physical states for mode  $A$ , namely a state with no bosons and a state with one boson, even though the contributions  $\hat{\rho}_1^A$  and  $\hat{\rho}_2^A$  are non physical states consisting of pure states that are each quantum superpositions of a zero boson state and a one boson state - in violation of the super-selection rule. However even a minute change in the  $P_R$  will lead to the reduced density operators  $\hat{\rho}_A, \hat{\rho}_B, \dots$  that are non physical. In the example given, changes to  $P_1 = 0.51$  and  $P_2 = 0.49$  will lead to non physical contributions  $|0\rangle_A \langle 1|_A$  and  $|1\rangle_A \langle 0|_A$  to the reduced density operator  $\hat{\rho}_A$ . Also, as *all* the reduced density operators must represent physical states, then the sums in  $\hat{\rho}_A = \sum_R P_R \hat{\rho}_R^A, \hat{\rho}_B = \sum_R P_R \hat{\rho}_R^B, \dots$  must *all* lead to physical states. Since the probabilities  $P_R$  depend on the preparation process that generates the mixed non-entangled state, and may for example depend on external parameters such as temperature, it would be extremely unlikely for given  $\hat{\rho}_R^A, \hat{\rho}_R^B, \dots$  that *all* such sums will lead to physical states, though for *special choices* of the mode density operators and the  $P_R$  this can occur. In addition, the density operators for the

other modes must be chosen so that the overall density operator is consistent with the super-selection rule. For example in the case where there are only two modes, the density operators  $\hat{\rho}_1^B = |0\rangle_B \langle 0|_B$  and  $\hat{\rho}_2^B = |1\rangle_B \langle 1|_B$  would lead to a physically valid reduced density operator  $\hat{\rho}_B = \frac{1}{2}(|0\rangle_B \langle 0|_B) + \frac{1}{2}(|1\rangle_B \langle 1|_B)$  for mode  $B$ , but there would be terms such as  $\frac{1}{4}|0\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B$  in the overall density operator, and such a term involves a coherence between an  $N = 0$  state and an  $N = 1$  state which is disallowed. Indeed, for the  $\hat{\rho}_1^A, \hat{\rho}_2^A$  and  $P_1, P_2$  as in Eq. (42), there may be no choice for  $\hat{\rho}_1^B$  and  $\hat{\rho}_2^B$  that gives rise to an overall physical state. In Appendix 13 the situation where  $\hat{\rho}_1^B$  and  $\hat{\rho}_2^B$  are associated with two general pure orthogonal states of the form  $\alpha|0\rangle_B + \beta|1\rangle_B$  and  $-\beta^*|0\rangle_B + \alpha^*|1\rangle_B$  with  $(|\alpha|^2 + |\beta|^2) = 1$ , is considered, and we find that no choice of  $\alpha$  and  $\beta$  leads to an overall physical state - although again the reduced density operator  $\hat{\rho}_B = \frac{1}{2}(|0\rangle_B \langle 0|_B) + \frac{1}{2}(|1\rangle_B \langle 1|_B)$  is physical.

### 2.9.6 Example of Global but not Local Particle Number SSR Compliant State

However, in some cases sub-system density operators can be chosen in the context of two mode systems which comply with the global particle number SSR but not the local particle number SSR. Such a case is presented by Verstraete et al [27], [28]. The overall density operator is a statistical mixture

$$\begin{aligned} \hat{\rho} = & \frac{1}{4}(|\psi_1\rangle \langle \psi_1|)_A \otimes |\psi_1\rangle \langle \psi_1|_B + \frac{1}{4}(|\psi_i\rangle \langle \psi_i|)_A \otimes |\psi_i\rangle \langle \psi_i|_B \\ & + \frac{1}{4}(|\psi_{-1}\rangle \langle \psi_{-1}|)_A \otimes |\psi_{-1}\rangle \langle \psi_{-1}|_B + \frac{1}{4}(|\psi_{-i}\rangle \langle \psi_{-i}|)_A \otimes |\psi_{-i}\rangle \langle \psi_{-i}|_B \end{aligned} \quad (44)$$

where  $|\psi_\omega\rangle = (|0\rangle + \omega|1\rangle)/\sqrt{2}$ , with  $\omega = 1, i, -, -i$ . The  $|\psi_\omega\rangle$  are superpositions of zero and one boson states and consequently the local particle number SSR is violated by each of the sub-system density operators  $|\psi_\omega\rangle \langle \psi_\omega|_A$  and  $|\psi_\omega\rangle \langle \psi_\omega|_B$ . On the other hand, the global particle number SSR is obeyed since the density operator can also be written as

$$\begin{aligned} \hat{\rho} = & \frac{1}{4}(|0\rangle \langle 0|)_A \otimes |0\rangle \langle 0|_B + \frac{1}{4}(|1\rangle \langle 1|)_A \otimes |1\rangle \langle 1|_B \\ & + \frac{1}{2}(|\Psi_+\rangle \langle \Psi_+|)_{AB} \end{aligned} \quad (45)$$

where  $|\Psi_+\rangle_{AB} = (|0\rangle_A |1\rangle_B + |1\rangle_A |0\rangle_B)/\sqrt{2}$ . This is a statistical mixture of  $N = 0, 1, 2$  boson states. Although the expression in Eq.(44) is of the form in Eq.(1), the subsystem density operators  $|\psi_\omega\rangle \langle \psi_\omega|_A$  and  $|\psi_\omega\rangle \langle \psi_\omega|_B$  do not comply with the local particle number SSR, so this paper the state would be regarded as entangled. However, Verstraete et al [27], [28] regard it as separable. They would call it separable but nonlocal.

### 2.9.7 General Form of Non-Entangled States

To summarise: basically the sub-systems are *single modes* that the identical bosons can occupy, the super-selection rule for identical bosons, massive or oth-

erwise, prohibits states which are coherent superpositions of states with different numbers of bosons, and the only physically allowable  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , ..for the separate mode sub-systems that are themselves compatible with the local particle number SSR are allowed. For single mode sub-systems these can be written as statistical mixtures of states with definite numbers of bosons in the form

$$\hat{\rho}_R^A = \sum_{n_A} P_{n_A}^A |n_A\rangle \langle n_A| \quad \hat{\rho}_R^B = \sum_{n_B} P_{n_B}^B |n_B\rangle \langle n_B| \quad .. \quad (46)$$

However, in cases where the sub-systems are *pairs of modes* the density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , ..for the separate sub-systems are still required to conform to the symmetrisation principle and the super-selection rule. The forms for  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , .. are now of course more complex, as entanglement *within* the pairs of modes  $A_1, A_2$  associated with sub-system  $A$ , the pairs of modes  $B_1, B_2$  associated with sub-system  $B$ , etc is now possible within the definition for the general non-entangled state Eq. (1) for these *pairs* of modes. Within each pair of modes  $A_1, A_2$  statistical mixtures of states with differing total numbers  $N_A$  bosons in the two modes are possible and the sub-system density operators are based on states of the form given in Eq. (29). We have

$$\begin{aligned} |\Phi_{N_A}\rangle_A &= \sum_{k=0}^{N_A} C_{A\Phi}(N_A, k) |k\rangle_{A_1} \otimes |N_A - k\rangle_{A_2} \\ \hat{\rho}_R^A &= \sum_{N_A=0}^{\infty} \sum_{\Phi} P_{\Phi N_A} |\Phi_{N_A}\rangle_A \langle \Phi_{N_A}|_A \end{aligned} \quad (47)$$

with analogous expressions for the density operators  $\hat{\rho}_R^B$  etc for the other pairs of modes. Note that  $|\Phi_{N_A}\rangle_A$  only involves quantum superpositions of states with the same total number of bosons  $N_A$ . The expression (157) in SubSection 5.3 is of this form.

## 2.10 Two Mode Coherent State Mixture

To further illustrate some of the points made about super-selection rules - local and global - it is useful to consider a specific case also presented by Verstraete et al [27], [28]. This *mixture of two mode coherent states* is represented by the two mode density operator

$$\begin{aligned} \hat{\rho} &= \int \frac{d\theta}{2\pi} |\alpha, \alpha\rangle \langle \alpha, \alpha| \\ &= \int \frac{d\theta}{2\pi} (|\alpha\rangle \langle \alpha|)_A \otimes (|\alpha\rangle \langle \alpha|)_B \end{aligned} \quad (48)$$

where  $|\alpha\rangle_C$  is a one mode coherent state for mode  $C = A, B$  with  $\alpha = |\alpha| \exp(-i\theta)$ , and modes  $A, B$  are associated with bosonic annihilation operators  $\hat{a}, \hat{b}$ . The magnitude  $|\alpha|$  is fixed.

This density operator *appears* to be that for a non-entangled state of modes  $A, B$  in the form

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B \quad (49)$$

with  $\sum_R P_R \rightarrow \int \frac{d\theta}{2\pi}$  and  $\hat{\rho}_R^A \rightarrow (|\alpha\rangle\langle\alpha|)_A$  and  $\hat{\rho}_R^B \rightarrow (|\alpha\rangle\langle\alpha|)_B$ . However although this choice of  $\hat{\rho}_R^A, \hat{\rho}_R^B$  satisfy the Hermitiancy, unit trace, positivity features they do *not* conform to the requirement of satisfying the (*local*) sub-system boson number *super-selection rule*. From Eq. (48) we have

$$\begin{aligned} \langle n | (|\alpha\rangle\langle\alpha|) | m \rangle_A &= \exp(-|\alpha|^2) \frac{\alpha^n}{\sqrt{n!}} \frac{(\alpha)^{*m}}{\sqrt{m!}} \\ \langle p | (|\alpha\rangle\langle\alpha|) | q \rangle_B &= \exp(-|\alpha|^2) \frac{\alpha^p}{\sqrt{p!}} \frac{(\alpha)^{*q}}{\sqrt{q!}} \end{aligned} \quad (50)$$

so clearly for each of the separate modes there are *coherences* between Fock states with differing boson occupation numbers. In the approach in the present paper the density operator in Eq. (48) does *not* represent a non-entangled state. However, in the papers of Verstraete et al [27], [28], Hillery et al [29], [30] and others it would represent an allowable non-entangled (separable) state. Indeed, Verstraete et al [27] specifically state "... this state is *obviously* separable, though the states  $|\alpha\rangle$  are incompatible with the (local) super-selection rule.". Verstraete et al [27] introduce the state defined in Eq. (48) as an example of a state that is separable (in their terms) but which cannot be prepared locally, because it is incompatible with the local particle number super-selection rule.

The *mixture* of *two mode coherent states* does of course satisfy the *total* or *global* boson number super-selection rule. The matrix elements between two mode Fock states are

$$\begin{aligned} (\langle n |_A \otimes \langle p |_B) \hat{\rho} (|m\rangle_A \otimes |q\rangle_B) &= \exp(-2|\alpha|^2) \frac{|\alpha|^{n+m}}{\sqrt{n!}\sqrt{m!}} \frac{|\alpha|^{p+q}}{\sqrt{p!}\sqrt{q!}} \int \frac{d\theta}{2\pi} \exp(-i(n-m+p-q)\theta) \\ &= \exp(-2|\alpha|^2) \frac{|\alpha|^{n+m}}{\sqrt{n!}\sqrt{m!}} \frac{|\alpha|^{p+q}}{\sqrt{p!}\sqrt{q!}} \delta_{n+p, m+q} \end{aligned} \quad (51)$$

These overall matrix elements are zero unless  $n+p = m+q$ , showing that there are *no coherences* between two mode Fock states where the total boson number differs. The mixture of two mode coherent states has the interesting feature of providing an example of a two mode state which satisfies the global but not the local super-selection rule.

The *reduced density operators* for modes  $A, B$  are

$$\hat{\rho}_A = \int \frac{d\theta}{2\pi} (|\alpha\rangle\langle\alpha|)_A \quad \hat{\rho}_B = \int \frac{d\theta}{2\pi} (|\alpha\rangle\langle\alpha|)_B$$

and a straightforward calculation gives

$$\hat{\rho}_A = \exp(-|\alpha|^2) \sum_n \frac{|\alpha|^{2n}}{n!} (|n\rangle\langle n|)_A \quad \hat{\rho}_B = \exp(-|\alpha|^2) \sum_p \frac{|\alpha|^{2p}}{p!} (|p\rangle\langle p|)_B$$

which are statistical mixtures of Fock states with the expected Poisson distribution associated with coherent states. This shows that the reduced density operators *are* consistent with the separate mode local super-selection rule, whereas the density operators  $\hat{\rho}_R^A = (|\alpha\rangle\langle\alpha|)_A$ ,  $\hat{\rho}_R^B = (|\alpha\rangle\langle\alpha|)_B$  are *not*. Later we will revisit this example in the context of entanglement tests.

## 2.11 Two Mode System - Coherence Terms

The general non-entangled state for modes  $\hat{a}$  and  $\hat{b}$  is given by

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B \quad (52)$$

and as a consequence of the requirement that  $\hat{\rho}_R^A$  and  $\hat{\rho}_R^B$  are physical states for modes  $\hat{a}$  and  $\hat{b}$  satisfying the super-selection rule, it follows that

$$\begin{aligned} \langle (\hat{a})^n \rangle_a &= Tr(\hat{\rho}_R^A (\hat{a})^n) = 0 & \langle (\hat{a}^\dagger)^n \rangle_a &= Tr(\hat{\rho}_R^A (\hat{a}^\dagger)^n) = 0 \\ \langle (\hat{b})^m \rangle_b &= Tr(\hat{\rho}_R^B (\hat{b})^m) = 0 & \langle (\hat{b}^\dagger)^m \rangle_b &= Tr(\hat{\rho}_R^B (\hat{b}^\dagger)^m) = 0 \end{aligned} \quad (53)$$

Thus coherence terms are zero. As we will see these results will limit spin squeezing to entangled states of modes  $\hat{a}$  and  $\hat{b}$ . Note that similar results also apply when non-entangled states for the original modes  $\hat{c}$  and  $\hat{d}$  are considered -  $\langle (\hat{c})^n \rangle_c = 0$ , etc..

## 2.12 Two Sub-Systems of Pairs of Modes - Coherence Terms

In this case the general non-entangled state where  $A$  and  $B$  are pairs of modes -  $A_1, A_2$  associated with sub-system  $A$ , and modes  $B_1, B_2$  associated with sub-system  $B$ , the overall density operator is of the form (74), with  $C \rightarrow A$ ,  $D \rightarrow B$ , whilst the sub-system density operators are of the forms given in (47). In this case we now have in general

$$\begin{aligned} \langle (\hat{a}_i)^n \rangle_A &= Tr(\hat{\rho}_R^A (\hat{a}_i)^n) \neq 0 & \langle (\hat{a}_i^\dagger)^n \rangle_A &= Tr(\hat{\rho}_R^A (\hat{a}_i^\dagger)^n) \neq 0 \\ \langle (\hat{b}_j)^m \rangle_B &= Tr(\hat{\rho}_R^B (\hat{b}_j)^m) \neq 0 & \langle (\hat{b}_j^\dagger)^m \rangle_B &= Tr(\hat{\rho}_R^B (\hat{b}_j^\dagger)^m) \neq 0 \\ i, j &= 1, 2 \end{aligned} \quad (54)$$

so unlike the case where the two sub-systems are single modes, there are non-zero coherences when they are pairs of modes.

### 3 Spin Squeezing

The basic concept of spin squeezing was first introduced by Kitagawa and Ueda [40] for general spin systems. These include cases based on two mode systems, such as may occur both for optical fields and for Bose-Einstein condensates. Though focused on systems of massive identical bosons, the treatment in this paper also applies to photons though details will differ.

#### 3.1 Spin Operators, Bloch Vector and Covariance Matrix

##### 3.1.1 Spin Operators

For two mode systems with mode annihilation operators  $\hat{a}$ ,  $\hat{b}$  associated with the two single particle states  $|\phi_a\rangle$ ,  $|\phi_b\rangle$ , and where the non-zero bosonic commutation rules are  $[\hat{e}, \hat{e}^\dagger] = \hat{1}$  ( $\hat{e} = \hat{a}$  or  $\hat{b}$ ), Schwinger *spin angular momentum operators*  $\hat{S}_\xi$  ( $\xi = x, y, z$ ) are defined as

$$\hat{S}_x = (\hat{b}^\dagger \hat{a} + \hat{a}^\dagger \hat{b})/2 \quad \hat{S}_y = (\hat{b}^\dagger \hat{a} - \hat{a}^\dagger \hat{b})/2i \quad \hat{S}_z = (\hat{b}^\dagger \hat{b} - \hat{a}^\dagger \hat{a})/2 \quad (55)$$

and which satisfy the commutation rules  $[\hat{S}_\xi, \hat{S}_\mu] = i\epsilon_{\xi\mu\lambda}\hat{S}_\lambda$  for angular momentum operators. For bosons the square of the angular momentum operators is given by  $\hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = (\hat{N}/2)(\hat{N}/2 + 1)$ , where  $\hat{N} = (\hat{b}^\dagger \hat{b} + \hat{a}^\dagger \hat{a})$  is the boson total number operator, those for the separate modes being  $\hat{n}_e = \hat{e}^\dagger \hat{e}$  ( $\hat{e} = \hat{a}$  or  $\hat{b}$ ). The Schwinger spin operators are the second quantization form of symmetrized one body operators  $\hat{S}_x = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| + |\phi_a(i)\rangle \langle \phi_b(i)|)/2$ ;  $\hat{S}_y = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| - |\phi_a(i)\rangle \langle \phi_b(i)|)/2i$ ;  $\hat{S}_z = \sum_i (|\phi_b(i)\rangle \langle \phi_b(i)| - |\phi_a(i)\rangle \langle \phi_a(i)|)/2$ , where the sum  $i$  is over the identical bosonic particles. In the case of the two mode EM field the spin angular momentum operators are related to the Stokes parameters.

##### 3.1.2 Bloch Vector and Covariance Matrix

If the density operator for the overall system is  $\hat{\rho}$  then expectation values of the three spin operators  $\langle \hat{S}_\xi \rangle = \text{Tr}(\hat{\rho} \hat{S}_\xi)$  ( $\xi = x, y, z$ ) define the *Bloch vector*. Spin squeezing is related to the fluctuation operators  $\Delta \hat{S}_\xi = \hat{S}_\xi - \langle \hat{S}_\xi \rangle$ , in terms of which a real, symmetric *covariance matrix*  $C(\hat{S}_\xi, \hat{S}_\mu)$  ( $\xi, \mu = x, y, z$ ) is defined [64], [56] via

$$\begin{aligned} C(\hat{S}_\xi, \hat{S}_\mu) &= (\langle \Delta \hat{S}_\xi \Delta \hat{S}_\mu \rangle + \langle \Delta \hat{S}_\mu \Delta \hat{S}_\xi \rangle)/2 \\ &= \langle \hat{S}_\xi \hat{S}_\mu + \hat{S}_\mu \hat{S}_\xi \rangle / 2 - \langle \hat{S}_\xi \rangle \langle \hat{S}_\mu \rangle \end{aligned} \quad (56)$$

and whose diagonal elements  $C(\hat{S}_\xi, \hat{S}_\xi) = \langle \Delta \hat{S}_\xi^2 \rangle$  gives the variance for the fluctuation operators. The variances for the spin operators satisfy the three Heisenberg uncertainty principle relations  $\langle \Delta \hat{S}_x^2 \rangle \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{4} |\langle \hat{S}_z \rangle|^2$ ;  $\langle \Delta \hat{S}_y^2 \rangle \langle \Delta \hat{S}_z^2 \rangle \geq$

$\frac{1}{4}|\langle \hat{S}_x \rangle|^2$ ;  $\langle \Delta \hat{S}_z^2 \rangle \langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{4}|\langle \hat{S}_y \rangle|^2$ , and spin squeezing is usually defined via conditions such as  $\langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2}|\langle \hat{S}_z \rangle|$  with  $\langle \Delta \hat{S}_y^2 \rangle > \frac{1}{2}|\langle \hat{S}_z \rangle|$ , for  $\hat{S}_x$  being squeezed compared to  $\hat{S}_y$  and so on. However this definition is unsatisfactory since it ignores the presence of the off-diagonal elements of the covariance matrix, so a better definition is required.

### 3.2 New Spin Operators and Principal Spin Fluctuations

The covariance matrix has real, non-negative eigenvalues and can be diagonalised via an orthogonal *rotation matrix*  $M(-\alpha, -\beta, -\gamma)$  that defines *new spin angular momentum operators*  $\hat{J}_\xi$  ( $\xi = x, y, z$ ) via

$$\hat{J}_\xi = \sum_{\mu} M_{\xi\mu}(-\alpha, -\beta, -\gamma) \hat{S}_\mu \quad (57)$$

and where

$$\begin{aligned} C(\hat{J}_\xi, \hat{J}_\mu) &= \sum_{\lambda\theta} M_{\xi\lambda}(-\alpha, -\beta, -\gamma) C(\hat{S}_\lambda, \hat{S}_\theta) M_{\mu\theta}(-\alpha, -\beta, -\gamma) \\ &= \delta_{\xi\mu} \langle \Delta \hat{J}_\xi^2 \rangle \end{aligned} \quad (58)$$

is the covariance matrix for the new spin angular momentum operators  $\hat{J}_\xi$  ( $\xi = x, y, z$ ), and which is *diagonal* with the diagonal elements  $\langle \Delta \hat{J}_x^2 \rangle$ ,  $\langle \Delta \hat{J}_y^2 \rangle$  and  $\langle \Delta \hat{J}_z^2 \rangle$  giving the so-called *principal spin fluctuations*. The matrix  $M(\alpha, \beta, \gamma)$  is parameterised in terms of three Euler angles  $\alpha, \beta, \gamma$  and is given in [65] (see Eq. (4.43)).

The Bloch vector and spin fluctuations are illustrated in Figure 1. In Fig 1 the Bloch vector and spin fluctuation ellipsoid is shown in terms of the original spin operators  $\hat{S}_\xi$  ( $\xi = x, y, z$ )

Figure 1 near here.

### 3.3 Spin Squeezing for New Spin Operators

#### 3.3.1 Heisenberg Uncertainty Principle and Spin Squeezing

Since the new spin operators also satisfy *Heisenberg uncertainty principle* relationships

$$\begin{aligned} \langle \Delta \hat{J}_x^2 \rangle \langle \Delta \hat{J}_y^2 \rangle &\geq \frac{1}{4} |\langle \hat{J}_z \rangle|^2 \\ \langle \Delta \hat{J}_y^2 \rangle \langle \Delta \hat{J}_z^2 \rangle &\geq \frac{1}{4} |\langle \hat{J}_x \rangle|^2 \\ \langle \Delta \hat{J}_z^2 \rangle \langle \Delta \hat{J}_x^2 \rangle &\geq \frac{1}{4} |\langle \hat{J}_y \rangle|^2 \end{aligned} \quad (59)$$

*spin squeezing* will now be defined via conditions such as

$$\begin{aligned}\langle \Delta \hat{J}_x^2 \rangle &< \frac{1}{2} |\langle \hat{J}_z \rangle| \text{ and } \langle \Delta \hat{J}_y^2 \rangle > \frac{1}{2} |\langle \hat{J}_z \rangle| \\ \langle \Delta \hat{J}_y^2 \rangle &< \frac{1}{2} |\langle \hat{J}_x \rangle| \text{ and } \langle \Delta \hat{J}_z^2 \rangle > \frac{1}{2} |\langle \hat{J}_x \rangle| \\ \langle \Delta \hat{J}_z^2 \rangle &< \frac{1}{2} |\langle \hat{J}_y \rangle| \text{ and } \langle \Delta \hat{J}_x^2 \rangle > \frac{1}{2} |\langle \hat{J}_y \rangle|\end{aligned}\quad (60)$$

for  $\hat{J}_x$  being squeezed compared to  $\hat{J}_y$ , and so on. By convention we may choose  $\langle \Delta \hat{J}_x^2 \rangle \leq \langle \Delta \hat{J}_y^2 \rangle \leq \langle \Delta \hat{J}_z^2 \rangle$ , so the primary spin operator of interest will be  $\hat{J}_x$  since this has the smallest fluctuation. Note that here we have chosen principal spin fluctuations, but of course the last Heisenberg uncertainty relations apply for *any* new choice of rotated spin operators - as occurs in the next part of this section.

### 3.3.2 Alternative Spin Squeezing Criteria

*Other criteria* for spin squeezing are also used, for example in the article by Wineland et al [66]. To focus on spin squeezing for  $\hat{J}_x$  compared to *any* orthogonal spin operators we can combine the first and third Heisenberg uncertainty principle relationships to give

$$\langle \Delta \hat{J}_x^2 \rangle \left( \langle \Delta \hat{J}_y^2 \rangle + \langle \Delta \hat{J}_z^2 \rangle \right) \geq \frac{1}{4} \left( |\langle \hat{J}_y \rangle|^2 + |\langle \hat{J}_z \rangle|^2 \right) \quad (61)$$

Then we may define two new spin operators via

$$\hat{J}_{\perp 1} = \cos \theta \hat{J}_y + \sin \theta \hat{J}_z \quad \hat{J}_{\perp 2} = -\sin \theta \hat{J}_y + \cos \theta \hat{J}_z \quad (62)$$

where  $\theta$  corresponds to a rotation angle in the  $yz$  plane, and which satisfy the standard angular momentum commutation rules  $[\hat{J}_{\perp 1}, \hat{J}_{\perp 2}] = i\hat{J}_x$ ,  $[\hat{J}_{\perp 2}, \hat{J}_x] = i\hat{J}_{\perp 1}$ ,  $[\hat{J}_x, \hat{J}_{\perp 1}] = i\hat{J}_{\perp 2}$ . It is straightforward to show that  $\langle \Delta \hat{J}_y^2 \rangle + \langle \Delta \hat{J}_z^2 \rangle = \langle \Delta \hat{J}_{\perp 1}^2 \rangle + \langle \Delta \hat{J}_{\perp 2}^2 \rangle$  and  $|\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2 = |\langle \hat{J}_y \rangle|^2 + |\langle \hat{J}_z \rangle|^2$  so that

$$\langle \Delta \hat{J}_x^2 \rangle \left( \langle \Delta \hat{J}_{\perp 1}^2 \rangle + \langle \Delta \hat{J}_{\perp 2}^2 \rangle \right) \geq \frac{1}{4} \left( |\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2 \right) \quad (63)$$

so that *spin squeezing* for  $\hat{J}_x$  compared to *any two* orthogonal spin operators such as  $\hat{J}_{\perp 1}$  or  $\hat{J}_{\perp 2}$  would be defined as

$$\begin{aligned}\langle \Delta \hat{J}_x^2 \rangle &< \frac{1}{2} \sqrt{(|\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2)} \\ \text{and} \\ \langle \Delta \hat{J}_{\perp 1}^2 \rangle + \langle \Delta \hat{J}_{\perp 2}^2 \rangle &> \frac{1}{2} \sqrt{(|\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2)}\end{aligned}\quad (64)$$



This criterion would apply however the choice of rotation matrix  $M(-\alpha, -\beta, -\gamma)$  is made, so  $\Delta\hat{J}_x$  does not have to correspond to the principal spin fluctuation with the smallest variance though obviously such a choice is preferable over some arbitrary set of new spin operators. For spin squeezing in  $\langle\Delta\hat{J}_x^2\rangle$  we require

$$\xi^2 = \frac{\langle\Delta\hat{J}_x^2\rangle}{(|\langle\hat{J}_{\perp 1}\rangle|^2 + |\langle\hat{J}_{\perp 2}\rangle|^2)} < \frac{1}{2\sqrt{(|\langle\hat{J}_{\perp 1}\rangle|^2 + |\langle\hat{J}_{\perp 2}\rangle|^2)}} \sim \frac{1}{N} \quad (65)$$

The last step is an approximation based on the assumption that the Bloch vector lies in the  $yz$  plane and close to the Bloch sphere, this situation being the most conducive to detecting the fluctuation  $\langle\Delta\hat{J}_x^2\rangle$ . In this situation  $\sqrt{(|\langle\hat{J}_{\perp 1}\rangle|^2 + |\langle\hat{J}_{\perp 2}\rangle|^2)}$  is approximately  $N/2$ . The condition  $\xi^2 < 1/N$  is sometimes taken as the condition for spin squeezing [67], but it should be noted that this is approximate and Eq. (64) gives the correct expression.

### 3.3.3 Planar Spin Squeezing

A special case of recent interest is that referred to as *planar squeezing* [68] in which the Bloch vector for a suitable choice of spin operators lies in a *plane* and along one of the *axes*. If this plane is chosen to be the  $xy$  plane and the  $x$  axis is chosen then  $\langle\hat{J}_z\rangle = 0$  and  $\langle\hat{J}_y\rangle = 0$ , resulting in only one Heisenberg uncertainty principle relationship where the right side is non-zero, namely  $\langle\Delta\hat{J}_y^2\rangle\langle\Delta\hat{J}_z^2\rangle \geq \frac{1}{4}|\langle\hat{J}_x\rangle|^2$ . Combining this with  $\langle\Delta\hat{J}_x^2\rangle\langle\Delta\hat{J}_y^2\rangle \geq 0$  gives  $(\langle\Delta\hat{J}_y^2\rangle + \langle\Delta\hat{J}_x^2\rangle)\langle\Delta\hat{J}_z^2\rangle \geq \frac{1}{4}|\langle\hat{J}_x\rangle|^2$ . So the total spin fluctuation in the  $xy$  plane defined as  $\langle\Delta\hat{J}_{\parallel}^2\rangle = \langle\Delta\hat{J}_y^2\rangle + \langle\Delta\hat{J}_x^2\rangle$  will be squeezed compared to the total spin fluctuation perpendicular to the  $xy$  plane given by  $\langle\Delta\hat{J}_{\perp}^2\rangle = \langle\Delta\hat{J}_z^2\rangle$  if

$$\langle\Delta\hat{J}_{\parallel}^2\rangle < \frac{1}{2}|\langle\hat{J}_x\rangle| \text{ and } \langle\Delta\hat{J}_{\perp}^2\rangle > \frac{1}{2}|\langle\hat{J}_x\rangle| \quad (66)$$

By minimising  $\langle\Delta\hat{J}_{\parallel}^2\rangle$  whilst satisfying the constraints  $\langle\hat{J}_z\rangle = \langle\hat{J}_y\rangle = 0$  a spin squeezed state is found that satisfies (66) with  $\langle\Delta\hat{J}_{\parallel}^2\rangle \sim J^{2/3}$ ,  $\langle\Delta\hat{J}_{\perp}^2\rangle \sim J^{4/3}$ ,  $|\langle\hat{J}_x\rangle| \sim J$  for large  $J = N/2$  [68]. The Bloch vector is on the Bloch sphere and condition (65) is also satisfied.

### 3.4 Rotation Operators and New Modes

#### 3.4.1 Rotation Operators

The new spin operators are also related to the original spin operators via a *unitary rotation operator*  $\hat{R}(\alpha, \beta, \gamma)$  parameterised in terms of Euler angles so that

$$\hat{J}_\xi = \hat{R}(\alpha, \beta, \gamma) \hat{S}_\xi \hat{R}(\alpha, \beta, \gamma)^{-1} \quad (67)$$

where

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}_z(\alpha) \hat{R}_y(\beta) \hat{R}_z(\gamma) \quad (68)$$

with  $\hat{R}_\xi(\phi) = \exp(i\phi\hat{S}_\xi)$  describing a rotation about the  $\xi$  axis anticlockwise through an angle  $\phi$ . Details for the rotation operators and matrices are set out in [56]. Note that Eq. (67) specifies a rotation of the vector spin operator rather than a rotation of the axes, so  $\hat{J}_\xi$  ( $\xi = x, y, z$ ) are the components of the rotated vector spin operator with respect to the original axes.

#### 3.4.2 New Mode Operators

We can also see that the new spin operators are related to *new mode operators*  $\hat{c}$  and  $\hat{d}$  via

$$\hat{J}_x = (\hat{d}^\dagger \hat{c} + \hat{c}^\dagger \hat{d})/2 \quad \hat{J}_y = (\hat{d}^\dagger \hat{c} - \hat{c}^\dagger \hat{d})/2i \quad \hat{J}_z = (\hat{d}^\dagger \hat{d} - \hat{c}^\dagger \hat{c})/2 \quad (69)$$

where

$$\hat{c} = \hat{R}(\alpha, \beta, \gamma) \hat{a} \hat{R}(\alpha, \beta, \gamma)^{-1} \quad \hat{d} = \hat{R}(\alpha, \beta, \gamma) \hat{b} \hat{R}(\alpha, \beta, \gamma)^{-1} \quad (70)$$

For the bosonic case a straight-forward calculation gives the new mode operators as

$$\begin{aligned} \hat{c} &= \exp\left(\frac{1}{2}i\gamma\right) \left( \cos\left(\frac{\beta}{2}\right) \exp\left(\frac{1}{2}i\alpha\right) \hat{a} + \sin\left(\frac{\beta}{2}\right) \exp\left(-\frac{1}{2}i\alpha\right) \hat{b} \right) \\ \hat{d} &= \exp\left(-\frac{1}{2}i\gamma\right) \left( -\sin\left(\frac{\beta}{2}\right) \exp\left(\frac{1}{2}i\alpha\right) \hat{a} + \cos\left(\frac{\beta}{2}\right) \exp\left(-\frac{1}{2}i\alpha\right) \hat{b} \right) \end{aligned} \quad (71)$$

and it is easy to then check that  $\hat{c}$  and  $\hat{d}$  satisfy the expected non-zero bosonic commutation rules are  $[\hat{c}, \hat{c}^\dagger] = 1$  ( $\hat{c} = \hat{c}$  or  $\hat{d}$ ) and that the *total boson number operator* is  $\hat{N} = (\hat{d}^\dagger \hat{d} + \hat{c}^\dagger \hat{c})$ . As  $\hat{N}$  is invariant under unitary rotation operators it follows that  $\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = (\hat{N}/2)(\hat{N}/2 + 1)$ .

### 3.4.3 New Modes

The new mode operators correspond to *new single particle states*  $|\phi_c\rangle$ ,  $|\phi_d\rangle$  where

$$\begin{aligned} |\phi_c\rangle &= \exp(-\frac{1}{2}i\gamma) \left( \cos(\frac{\beta}{2}) \exp(-\frac{1}{2}i\alpha) |\phi_a\rangle + \sin(\frac{\beta}{2}) \exp(\frac{1}{2}i\alpha) |\phi_b\rangle \right) \\ |\phi_d\rangle &= \exp(\frac{1}{2}i\gamma) \left( -\sin(\frac{\beta}{2}) \exp(-\frac{1}{2}i\alpha) |\phi_a\rangle + \cos(\frac{\beta}{2}) \exp(\frac{1}{2}i\alpha) |\phi_b\rangle \right) \end{aligned} \quad (72)$$

These are two orthonormal quantum superpositions of the original single particle states  $|\phi_a\rangle$ ,  $|\phi_b\rangle$ , and as such represent an *alternative choice* of modes that could be realised experimentally.

Eqs. (71) can be inverted to give the old mode operators via

$$\begin{aligned} \hat{a} &= \exp(-\frac{1}{2}i\alpha) \left( \cos(\frac{\beta}{2}) \exp(-\frac{1}{2}i\gamma) \hat{c} - \sin(\frac{\beta}{2}) \exp(+\frac{1}{2}i\gamma) \hat{d} \right) \\ \hat{b} &= \exp(+\frac{1}{2}i\alpha) \left( \sin(\frac{\beta}{2}) \exp(\frac{1}{2}i\gamma) \hat{c} + \cos(\frac{\beta}{2}) \exp(-\frac{1}{2}i\gamma) \hat{d} \right) \end{aligned} \quad (73)$$

### 3.5 Two Mode System - Coherence Terms

For our two-mode case we have also seen that the original choice of modes with annihilation operators  $\hat{a}$  and  $\hat{b}$  may be replaced by new modes with annihilation operators  $\hat{c}$  and  $\hat{d}$ . Since the new modes are associated with new spin operators  $\hat{J}_\xi$  ( $\xi = x, y, z$ ) for which the covariance matrix is diagonal and where the diagonal elements give the variances that are relevant for the definition of spin squeezing, it is therefore more relevant to consider entanglement for the case where the sub-systems are modes  $\hat{c}$  and  $\hat{d}$ , rather than  $\hat{a}$  and  $\hat{b}$ . Consequently the general non-entangled state for modes  $\hat{c}$  and  $\hat{d}$  is given by

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^C \otimes \hat{\rho}_R^D \quad (74)$$

and as a consequence of the requirement that  $\hat{\rho}_R^C$  and  $\hat{\rho}_R^D$  are physical states for modes  $\hat{c}$  and  $\hat{d}$  satisfying the super-selection rule, it follows that

$$\begin{aligned} \langle (\hat{c})^n \rangle_c &= \text{Tr}(\hat{\rho}_R^C (\hat{c})^n) = 0 & \langle (\hat{c}^\dagger)^n \rangle_c &= \text{Tr}(\hat{\rho}_R^C (\hat{c}^\dagger)^n) = 0 \\ \langle (\hat{d})^m \rangle_d &= \text{Tr}(\hat{\rho}_R^D (\hat{d})^m) = 0 & \langle (\hat{d}^\dagger)^m \rangle_d &= \text{Tr}(\hat{\rho}_R^D (\hat{d}^\dagger)^m) = 0 \end{aligned} \quad (75)$$

Thus coherence terms are zero. As we will see these results will limit spin squeezing to entangled states of modes  $\hat{c}$  and  $\hat{d}$ .

### 3.6 Quantum Correlation Functions and Measurements

Finally, we note that the principal spin fluctuations can be related to *quantum correlation functions*. For example, it is easy to show that

$$\begin{aligned} \langle \Delta \hat{J}_x^2 \rangle &= \frac{1}{4} \left( \langle (\hat{d}^\dagger)^2 (\hat{c})^2 \rangle + \langle (\hat{c}^\dagger)^2 (\hat{d})^2 \rangle + 2 \langle \hat{d}^\dagger \hat{c}^\dagger \hat{c} \hat{d} \rangle + \langle \hat{d}^\dagger \hat{d} \rangle + \langle \hat{c}^\dagger \hat{c} \rangle \right) \\ &\quad - \frac{1}{4} \left( \langle (\hat{d}^\dagger \hat{c})^2 \rangle + \langle (\hat{c}^\dagger \hat{d})^2 \rangle + 2 \langle \hat{d}^\dagger \hat{c} \rangle \langle \hat{c}^\dagger \hat{d} \rangle \right) \end{aligned} \quad (76)$$

showing that  $\langle \Delta \hat{J}_x^2 \rangle$  is related to various first and second order quantum correlation functions. These can be measured experimentally and are given theoretically in terms of phase space integrals involving distribution functions to represent the density operator and phase space variables to represent the mode annihilation, creation operators.

## 4 Spin Squeezing as a Test for Entanglement

With the general non-entangled state now required to be such that the density operators for the individual sub-systems must represent physical states and conform to the super-selection rule, the consequential link between entanglement in two mode bosonic systems and spin squeezing can now be established. We first consider spin squeezing for the principal spin operators  $\hat{J}_x$ ,  $\hat{J}_y$ ,  $\hat{J}_z$  and entangled states of the related new modes  $\hat{c}$ ,  $\hat{d}$  and then spin squeezing for the original spin operators  $\hat{S}_x$ ,  $\hat{S}_y$ ,  $\hat{S}_z$  and entangled states of the original modes  $\hat{a}$ ,  $\hat{b}$ . Examples of entangled states that are not spin squeezed and states that are not entangled nor spin squeezed for one choice of mode sub-systems, but are entangled and spin squeezed for another choice are then presented.

### 4.1 Spin Squeezing Requires Entanglement

Firstly, the *variance* for a Hermitian operator  $\hat{\Omega}$  in a mixed state

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R \quad (77)$$

is always greater than or equal to the the average of the variances for the separate components

$$\langle \Delta \hat{\Omega}^2 \rangle \geq \sum_R P_R \langle \Delta \hat{\Omega}^2 \rangle_R \quad (78)$$

where  $\langle \Delta \hat{\Omega}^2 \rangle = \text{Tr}(\hat{\rho} \Delta \hat{\Omega}^2)$  with  $\Delta \hat{\Omega} = \hat{\Omega} - \langle \hat{\Omega} \rangle$  and  $\langle \Delta \hat{\Omega}^2 \rangle_R = \text{Tr}(\hat{\rho}_R \Delta \hat{\Omega}_R^2)$  with  $\Delta \hat{\Omega}_R = \hat{\Omega} - \langle \hat{\Omega} \rangle_R$ . The proof is straight-forward and given in Ref. [69].

#### 4.1.1 Cases of $\hat{J}_x$ and $\hat{J}_y$

Next we calculate  $\langle \Delta \hat{J}_x^2 \rangle_R$ ,  $\langle \Delta \hat{J}_y^2 \rangle_R$  and  $\langle \hat{J}_x \rangle_R$ ,  $\langle \hat{J}_y \rangle_R$ ,  $\langle \hat{J}_z \rangle_R$  for the case where  $\hat{\rho}_R = \hat{\rho}_R^c \otimes \hat{\rho}_R^d$ . From Eqs. (69) we find that

$$\begin{aligned} \hat{J}_x^2 &= \frac{1}{4}((\hat{d}^\dagger)^2(\hat{c})^2 + \hat{d}^\dagger \hat{d} \hat{c} \hat{c}^\dagger + \hat{c}^\dagger \hat{c} \hat{d} \hat{d}^\dagger + (\hat{d})^2(\hat{c}^\dagger)^2) \\ \hat{J}_y^2 &= -\frac{1}{4}((\hat{d}^\dagger)^2(\hat{c})^2 - \hat{d}^\dagger \hat{d} \hat{c} \hat{c}^\dagger - \hat{c}^\dagger \hat{c} \hat{d} \hat{d}^\dagger + (\hat{d})^2(\hat{c}^\dagger)^2) \end{aligned} \quad (79)$$

so that on taking the trace with  $\hat{\rho}_R$  and using Eqs. (75) we get after applying the commutation rules  $[\hat{e}, \hat{e}^\dagger] = \hat{1}$  ( $\hat{e} = \hat{c}$  or  $\hat{d}$ )

$$\begin{aligned} \langle \hat{J}_x^2 \rangle_R &= \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R) \\ \langle \hat{J}_y^2 \rangle_R &= \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R) \end{aligned} \quad (80)$$

As we also have

$$\begin{aligned}\langle \hat{J}_x \rangle_R &= \frac{1}{2}(\langle \hat{d}^\dagger \rangle_R \langle \hat{c} \rangle_R + \langle \hat{c}^\dagger \rangle_R \langle \hat{d} \rangle_R) = 0 \\ \langle \hat{J}_y \rangle_R &= \frac{1}{2i}(\langle \hat{d}^\dagger \rangle_R \langle \hat{c} \rangle_R - \langle \hat{c}^\dagger \rangle_R \langle \hat{d} \rangle_R) = 0\end{aligned}\quad (81)$$

using Eqs. (75) and we see finally that the variances are

$$\begin{aligned}\langle \Delta \hat{J}_x^2 \rangle_R &= \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R) \\ \langle \Delta \hat{J}_y^2 \rangle_R &= \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R)\end{aligned}\quad (82)$$

and therefore from Eq. (78)

$$\begin{aligned}\langle \Delta \hat{J}_x^2 \rangle &\geq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R) \\ \langle \Delta \hat{J}_y^2 \rangle &\geq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R)\end{aligned}\quad (83)$$

Now

$$\langle \hat{J}_z \rangle = \sum_R P_R \frac{1}{2}(\langle \hat{d}^\dagger \hat{d} \rangle_R - \langle \hat{c}^\dagger \hat{c} \rangle_R) \quad (84)$$

so that

$$\frac{1}{2}|\langle \hat{J}_z \rangle| \leq \sum_R P_R \frac{1}{4}(|\langle \hat{d}^\dagger \hat{d} \rangle_R - \langle \hat{c}^\dagger \hat{c} \rangle_R|) \leq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) \quad (85)$$

and thus for any non-entangled state of modes  $\hat{c}$  and  $\hat{d}$

$$\begin{aligned}& \left| \langle \Delta \hat{J}_x^2 \rangle - \frac{1}{2}|\langle \hat{J}_z \rangle| \right| \\ & \geq \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) + \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R) - \sum_R P_R \frac{1}{4}(\langle \hat{d}^\dagger \hat{d} \rangle_R + \langle \hat{c}^\dagger \hat{c} \rangle_R) \\ & \geq \sum_R P_R \frac{1}{2}(\langle \hat{c}^\dagger \hat{c} \rangle_R \langle \hat{d}^\dagger \hat{d} \rangle_R) \\ & \geq 0\end{aligned}\quad (86)$$

Similar final steps show that  $|\langle \Delta \hat{J}_y^2 \rangle - \frac{1}{2}|\langle \hat{J}_z \rangle|| \geq 0$  for any non-entangled state of modes  $\hat{c}$  and  $\hat{d}$ .

This shows that for the general non-entangled state with modes  $\hat{c}$  and  $\hat{d}$  as the sub-systems, the variances for two of the principal spin fluctuations  $\langle \Delta \hat{J}_x^2 \rangle$  and  $\langle \Delta \hat{J}_y^2 \rangle$  are *both* greater than  $\frac{1}{2}|\langle \hat{J}_z \rangle|$ , and hence there is no spin squeezing for  $\hat{J}_x$  or  $\hat{J}_y$ . Note that as  $|\langle \hat{J}_y \rangle| = 0$ , the quantity  $\sqrt{(|\langle \hat{J}_{\perp 1} \rangle|^2 + |\langle \hat{J}_{\perp 2} \rangle|^2)}$

is the same as  $|\langle \hat{J}_z \rangle|$ , so the alternative criterion in Eq. (64) is the same as that in Eq. (60) which is used here.

We can extend the above to obtain further inequalities for the non-entangled state. Using Eq. (81)

$$\langle \hat{J}_x \rangle = \sum_R P_R \langle \hat{J}_x \rangle_R = 0 \quad \langle \hat{J}_y \rangle = \sum_R P_R \langle \hat{J}_y \rangle_R = 0 \quad (87)$$

it is easy to see that

$$\langle \Delta \hat{J}_x^2 \rangle - \frac{1}{2} |\langle \hat{J}_y \rangle| \geq 0 \quad \langle \Delta \hat{J}_y^2 \rangle - \frac{1}{2} |\langle \hat{J}_x \rangle| \geq 0 \quad (88)$$

for any non-entangled state of modes  $\hat{c}$  and  $\hat{d}$ . This completes the set of inequalities for the variances of  $\hat{J}_x$  and  $\hat{J}_y$ .

#### 4.1.2 Case of $\hat{J}_z$

For the other principal spin fluctuation we find that

$$\langle \Delta \hat{J}_z^2 \rangle_R = \frac{1}{4} \langle (\hat{d}^\dagger \hat{d} - \langle \hat{d}^\dagger \hat{d} \rangle_R) (\hat{d}^\dagger \hat{d} - \langle \hat{d}^\dagger \hat{d} \rangle_R) \rangle_R + \langle (\hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R) (\hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R) \rangle_R \quad (89)$$

so that using (78)

$$\langle \Delta \hat{J}_z^2 \rangle \geq \sum_R P_R \frac{1}{4} \langle (\hat{d}^\dagger \hat{d} - \langle \hat{d}^\dagger \hat{d} \rangle_R)^2 \rangle_R + \langle (\hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R)^2 \rangle_R \quad (90)$$

From Eq. (87) it follows that

$$\begin{aligned} & \langle \Delta \hat{J}_z^2 \rangle - \frac{1}{2} |\langle \hat{J}_x \rangle| \\ & \geq \sum_R P_R \frac{1}{4} \langle (\hat{d}^\dagger \hat{d} - \langle \hat{d}^\dagger \hat{d} \rangle_R)^2 \rangle_R + \langle (\hat{c}^\dagger \hat{c} - \langle \hat{c}^\dagger \hat{c} \rangle_R)^2 \rangle_R \\ & \geq 0 \end{aligned} \quad (91)$$

Similarly  $\langle \Delta \hat{J}_z^2 \rangle - \frac{1}{2} |\langle \hat{J}_y \rangle| \geq 0$ .

#### 4.1.3 No Spin Squeezing for Non-Entangled States

So overall, we have for the general non-entangled state of modes  $\hat{c}$  and  $\hat{d}$

$$\begin{aligned} \langle \Delta \hat{J}_x^2 \rangle & \geq \frac{1}{2} |\langle \hat{J}_z \rangle| \text{ and } \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle| \\ \langle \Delta \hat{J}_y^2 \rangle & \geq \frac{1}{2} |\langle \hat{J}_x \rangle| \text{ and } \langle \Delta \hat{J}_z^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_x \rangle| \\ \langle \Delta \hat{J}_z^2 \rangle & \geq \frac{1}{2} |\langle \hat{J}_y \rangle| \text{ and } \langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_y \rangle| \end{aligned} \quad (92)$$

Note that the last two pairs of inequalities are trivially true for the general non-entangled state, since  $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$ . This overall result tells us that for *any* non-entangled state of modes  $\hat{c}$  and  $\hat{d}$  we do *not* have  $\hat{J}_x$  being squeezed compared to  $\hat{J}_y$  (or vice-versa),  $\hat{J}_y$  being squeezed compared to  $\hat{J}_z$  (or vice-versa),  $\hat{J}_z$  being squeezed compared to  $\hat{J}_x$  (or vice-versa). That is, there is *no spin squeezing* for the non-entangled state!

#### 4.1.4 Spin Squeezing Tests for Entanglement

The key value of these results is the *spin squeezing test* for *entanglement* - if for a given state we find that

$$\text{If } \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle| \quad \text{or} \quad \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle| \quad (93)$$

or

$$\text{If } \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_x \rangle| \quad \text{or} \quad \langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} |\langle \hat{J}_x \rangle| \quad (94)$$

or

$$\text{If } \langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} |\langle \hat{J}_y \rangle| \quad \text{or} \quad \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} |\langle \hat{J}_y \rangle| \quad (95)$$

then the state *must* be entangled. Thus we only need to have spin squeezing in *any* of the  $\hat{J}_x$ ,  $\hat{J}_y$  or  $\hat{J}_z$  to demonstrate entanglement. No particular component need be singled out. Note that one cannot have both  $\langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle|$  and  $\langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle|$  etc. due to the Heisenberg uncertainty principle.

It is then straightforward to show that

$$\text{If } \langle \Delta \hat{J}_x^2 \rangle < \frac{1}{2} \sqrt{|\langle \hat{J}_{\perp 1}^x \rangle|^2 + |\langle \hat{J}_{\perp 2}^x \rangle|^2} \quad (96)$$

or

$$\text{If } \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} \sqrt{|\langle \hat{J}_{\perp 1}^y \rangle|^2 + |\langle \hat{J}_{\perp 2}^y \rangle|^2} \quad (97)$$

or

$$\text{If } \langle \Delta \hat{J}_z^2 \rangle < \frac{1}{2} \sqrt{|\langle \hat{J}_{\perp 1}^z \rangle|^2 + |\langle \hat{J}_{\perp 2}^z \rangle|^2} \quad (98)$$

that is, if  $\hat{J}_x$ ,  $\hat{J}_y$  or  $\hat{J}_z$  are squeezed compared to *any* of their two orthogonal spin components - then the state *must* be entangled. Again we only need to have spin squeezing in *any* of the  $\hat{J}_x$ ,  $\hat{J}_y$  or  $\hat{J}_z$  compared to *any* of their two orthogonal spin components to demonstrate entanglement.

#### 4.1.5 Inequality for $|\langle \hat{J}_z \rangle|$

Of the results for a *non-entangled* physical state for modes  $\hat{c}$  and  $\hat{d}$  we will later find it particularly important to consider the first of (92)

$$\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{J}_z \rangle| \quad (99)$$



This is because we can show that for any quantum state

$$|\langle \hat{J}_z \rangle| = \left| \left\langle \frac{1}{2}(\hat{n}_d - \hat{n}_c) \right\rangle \right| \leq \frac{1}{2}(|\langle \hat{n}_d \rangle| + |\langle \hat{n}_c \rangle|) = \frac{1}{2} \langle \hat{N} \rangle \quad (100)$$

there is an inequality involving  $|\langle \hat{J}_z \rangle|$  and the mean number of bosons  $\langle \hat{N} \rangle$  in the two mode system. Note that there *may* be entangled states for which  $\langle \Delta \hat{J}_x^2 \rangle$  and  $\langle \Delta \hat{J}_y^2 \rangle$  are both greater than  $\frac{1}{2}|\langle \hat{J}_z \rangle|$ , since all that has been proven is that for non-entangled states we must have *both*  $\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2}|\langle \hat{J}_z \rangle|$  and  $\langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{2}|\langle \hat{J}_z \rangle|$ .

Hence we may conclude that spin squeezing in either of the principal spin fluctuations  $\hat{J}_x$ ,  $\hat{J}_y$  or  $\hat{J}_z$  requires the quantum state to be entangled for the modes  $\hat{c}$  and  $\hat{d}$  as the sub-systems, these modes being associated with the principal spin fluctuations via Eq. (69). Although finding spin squeezing tells us that the state is entangled, there are however no simple relationships between the measures of entanglement and those of spin squeezing, so the linkage is essentially a qualitative one. For general quantum states, measures of entanglement for the specific situation of two sub-systems (bi-partite entanglement) are reviewed in [18].

## 4.2 Spin Squeezing requires Entanglement for Original Modes

It is also of some interest to consider spin squeezing for the original spin operators  $\hat{S}_x$ ,  $\hat{S}_y$ ,  $\hat{S}_z$  with the original modes  $\hat{a}$  and  $\hat{b}$  as the sub-systems, even though these spin operators are in general associated with a non-diagonal covariance matrix and the concept of spin squeezing is rather problematic in view of principal spin fluctuations not being involved. In this case the general non-entangled state for the *original* modes is given by

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B \quad (101)$$

with the  $\hat{\rho}_R^A$  and  $\hat{\rho}_R^B$  representing physical states for modes  $\hat{a}$  and  $\hat{b}$ , and where results analogous to Eqs. (75) apply. The same treatment applies as for spin operators  $\hat{J}_x$ ,  $\hat{J}_y$ ,  $\hat{J}_z$  with the modes  $\hat{c}$  and  $\hat{d}$  as the sub-systems and leads to the result for a *non-entangled* state of modes  $\hat{a}$  and  $\hat{b}$

$$\langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{2}|\langle \hat{S}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2}|\langle \hat{S}_z \rangle| \quad (102)$$

showing that neither  $\hat{S}_x$  or  $\hat{S}_y$  is spin squeezed for the general non-entangled state for modes  $\hat{a}$  and  $\hat{b}$  given in Eq. (101). We also have

$$\langle \hat{S}_x \rangle = \sum_R P_R \langle \hat{S}_x \rangle_R = 0 \quad \langle \hat{S}_y \rangle = \sum_R P_R \langle \hat{S}_y \rangle_R = 0 \quad (103)$$

so all the results analogous to Eqs. (92) also follow. Hence we may also conclude that spin squeezing in *any* of the original spin fluctuations requires the quantum state to be entangled when the original modes  $\hat{a}$  and  $\hat{b}$  are the sub-systems. Thus the *entanglement test* is

$$\text{If } \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle| \quad \text{or} \quad \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle| \quad (104)$$

or

$$\text{If } \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_x \rangle| \quad \text{or} \quad \langle \Delta \hat{S}_z^2 \rangle < \frac{1}{2} |\langle \hat{S}_x \rangle| \quad (105)$$

or

$$\text{If } \langle \Delta \hat{S}_z^2 \rangle < \frac{1}{2} |\langle \hat{S}_y \rangle| \quad \text{or} \quad \langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_y \rangle| \quad (106)$$

then we have an entangled state for the original modes  $\hat{a}$  and  $\hat{b}$ .

Hence we have seen that spin squeezing - either of the new or original spin operators requires entanglement of the new or original modes - the question then is: Does entanglement automatically lead to spin squeezing? The answer is no, since cases where the quantum state is entangled but not spin squeezed can be found. Thus in general, spin squeezing and entanglement are *not equivalent* - they do not occur *together* for all states. Spin squeezing is a *sufficient* condition for entanglement, it is not a *necessary* condition.

### 4.3 Entangled States that are Non Spin-Squeezed

One such example is the generalised  $N$  boson *NOON state* defined as

$$\begin{aligned} \hat{\rho} &= |\Phi\rangle \langle \Phi| \\ |\Phi\rangle &= \cos \theta \frac{(\hat{c}^\dagger)^N}{\sqrt{N!}} |0\rangle + \sin \theta \frac{(\hat{d}^\dagger)^N}{\sqrt{N!}} |0\rangle \\ &= \cos \theta \left| \frac{N}{2}, -\frac{N}{2} \right\rangle + \sin \theta \left| \frac{N}{2}, +\frac{N}{2} \right\rangle \end{aligned} \quad (107)$$

which is an entangled state for modes  $\hat{c}$  and  $\hat{d}$  in all cases except where  $\cos \theta$  or  $\sin \theta$  is zero. In the last form the state is expressed in terms of the eigenstates for  $(\hat{J}_x)^2$  and  $\hat{J}_z$ , as detailed in [56].

A straight-forward calculation gives

$$\begin{aligned} \langle \hat{J}_x \rangle &= 0 & \langle \hat{J}_y \rangle &= 0 & \langle \hat{J}_z \rangle &= -\frac{N}{2} \cos 2\theta \\ \langle \Delta \hat{J}_x^2 \rangle &= \frac{N}{4} & \langle \Delta \hat{J}_y^2 \rangle &= \frac{N}{4} & \langle \Delta \hat{J}_z^2 \rangle &= \frac{N^2}{4} (1 - \cos^2 2\theta) \end{aligned} \quad (108)$$

for  $N > 1$ , so that using the criteria for spin squeezing given in Eq. (60) we see that as  $\langle \Delta \hat{J}_x^2 \rangle - \frac{1}{2} |\langle \hat{J}_z \rangle| \geq 0$ , etc, and hence spin squeezing does not occur for this entangled state.

#### 4.4 Non-Entangled States that are Non Spin Squeezed

Of course from the previous section *any* non entangled state is definitely not spin squeezed. A specific example illustrating this is the  $N$  boson binomial state given by

$$\begin{aligned}\hat{\rho} &= |\Phi\rangle\langle\Phi| \\ |\Phi\rangle &= \frac{(-\hat{c}^\dagger)^N}{\sqrt{N!}} |0\rangle\end{aligned}\quad (109)$$

where  $\hat{c}$  and  $\hat{d}$  are given by Eqs. (71) with Euler angles  $\alpha = -\pi + \chi$ ,  $\beta = -2\theta$  and  $\gamma = -\pi$ , we find that

$$\begin{aligned}\hat{c} &= -\cos\theta \exp(\frac{1}{2}i\chi)\hat{a} - \sin\theta \exp(-\frac{1}{2}i\chi)\hat{b} = -\hat{a}_1 \\ \hat{d} &= \sin\theta \exp(\frac{1}{2}i\chi)\hat{a} - \cos\theta \exp(-\frac{1}{2}i\chi)\hat{b} = -\hat{a}_2\end{aligned}\quad (110)$$

where the mode operators  $\hat{a}_1$  and  $\hat{a}_2$  are as defined in [56] (see Eqs. (53) therein). The new spin angular momentum operators  $\hat{J}_\xi$  ( $\xi = x, y, z$ ) are the same as those defined in [56] (see Eqs. (64) therein) and in [56] it has been shown (see Eq. (60) therein) for the same binomial state as in (109) that

$$\begin{aligned}\langle\hat{J}_x\rangle &= 0 & \langle\hat{J}_y\rangle &= 0 & \langle\hat{J}_z\rangle &= -\frac{N}{2} \\ \langle\Delta\hat{J}_x^2\rangle &= \frac{N}{4} & \langle\Delta\hat{J}_y^2\rangle &= \frac{N}{4} & \langle\Delta\hat{J}_z^2\rangle &= 0\end{aligned}\quad (111)$$

(see Eqs. (162) and (176) therein). Hence the binomial state is not spin squeezed since  $\langle\Delta\hat{J}_x^2\rangle = \langle\Delta\hat{J}_y^2\rangle = \frac{1}{2}|\langle\hat{J}_z\rangle|$ . It is of course a *minimum uncertainty state* with spin fluctuations at the *standard quantum limit*. Clearly, it is a non-entangled state for modes  $\hat{c}$  and  $\hat{d}$ , being the product of a number state for mode  $\hat{c}$  with the vacuum state for mode  $\hat{d}$ .

Note that from the point of view of the original modes  $\hat{a}$  and  $\hat{b}$ , this is an entangled state. so the question is: Is it a spin squeezed state with respect to the original spin operators  $\hat{S}_\xi$  ( $\xi = x, y, z$ )? The Bloch vector and variances for this binomial state are given in [56] (see Eq. (163) in the main paper and Eq. (410) in the Appendix). The results include:

$$\begin{aligned}\langle\hat{S}_z\rangle &= -\frac{N}{2}\cos 2\theta \\ \langle\Delta\hat{S}_x^2\rangle &= \frac{N}{4}(\cos^2 2\theta \cos^2 \chi + \sin^2 \chi) & \langle\Delta\hat{S}_y^2\rangle &= \frac{N}{4}(\cos^2 2\theta \sin^2 \chi + \cos^2 \chi)\end{aligned}\quad (112)$$

This gives  $\langle\Delta\hat{S}_x^2\rangle\langle\Delta\hat{S}_y^2\rangle - \frac{1}{4}|\langle\hat{S}_z\rangle|^2 = \frac{1}{16}N^2(\cos^2 2\theta - 1)^2 \cos^2 \chi \sin^2 \chi \geq 0$  as required for the Heisenberg uncertainty principle. With  $\chi = 0$  we have

$\langle \Delta \hat{S}_x^2 \rangle = \frac{N}{4} \cos^2 2\theta$  and  $\langle \Delta \hat{S}_y^2 \rangle = \frac{N}{4}$ , whilst  $\frac{1}{2} |\langle \hat{S}_z \rangle| = \frac{N}{4} |\cos 2\theta|$ . As  $\langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle|$  there is spin squeezing in  $\hat{S}_x$  for this entangled state of modes  $\hat{a}$  and  $\hat{b}$ , though not of course for the new spin operator  $\hat{J}_x$  since this state is non-entangled for modes  $\hat{c}$  and  $\hat{d}$ . This example illustrates the need to carefully define spin squeezing and entanglement in terms of related sets of spin operators and modes. The same state is entangled with respect to one choice of modes - and spin squeezing occurs, whilst it is non-entangled with respect to another set of modes - and no spin squeezing occurs.

To summarise - with a physically based definition of non-entangled states for bosonic systems with two modes (related to the principal spin operators that have a diagonal covariance matrix) being the sub-systems and with a criterion for spin squeezing that focuses on these principal spin fluctuations, it seen that whilst non-entangled states are never spin squeezed and therefore although entanglement is a necessary condition for spin squeezing, it is not a sufficient one. There are entangled states that are not spin squeezed. Furthermore, as there is no simple quantitative links between measures of spin squeezing and those for entanglement, the mere presence of spin squeezing only demonstrates the qualitative result that the quantum state is entangled. Nevertheless, for high precision measurements based on spin operators where the primary emphasis is on how much spin squeezing can be achieved, knowing that entangled states are needed provides an impetus for studying such states and how they might be produced.

## 4.5 Entangled States that are Spin Squeezed

### 4.5.1 Relative Phase Eigenstate

As an example of an entangled state that is spin squeezed we consider the relative phase eigenstate  $|\frac{N}{2}, \theta_p\rangle$  for a two mode system in which there are  $N$  bosons. For modes with annihilation operators  $\hat{a}, \hat{b}$  the *relative phase eigenstate* is defined as

$$|\frac{N}{2}, \theta_p\rangle = \frac{1}{\sqrt{N+1}} \sum_{k=-N/2}^{N/2} \exp(ik\theta_p) \frac{(\hat{a}^\dagger)^{N/2-k}}{\sqrt{(N/2-k)!}} \frac{(\hat{b}^\dagger)^{N/2+k}}{\sqrt{(N/2+k)!}} |0\rangle \quad (113)$$

where the relative phase  $\theta_p = p(2\pi/(N+1))$  with  $p = -N/2, -N/2+1, \dots, +N/2$ , is an eigenvalue of the relative phase Hermitian operator of the type introduced by Barnett and Pegg [70] (see [56] and references therein). Note that the eigenvalues form a quasi-continuum over the range  $-\pi$  to  $+\pi$ , with a small separation between neighboring phases of  $O(1/N)$ . The relative phase state is consistent with the super-selection rule and is an entangled state for modes  $\hat{a}, \hat{b}$ . The Bloch vector for spin operators  $\hat{S}_x, \hat{S}_y, \hat{S}_z$  is given by (see [56])

$$\langle \hat{S}_x \rangle = N \frac{\pi}{8} \cos \theta_p \quad \langle \hat{S}_y \rangle = -N \frac{\pi}{8} \sin \theta_p \quad \langle \hat{S}_z \rangle = 0 \quad (114)$$

but the covariance matrix (see Eq. (178) in [56]) is non-diagonal.

#### 4.5.2 New Spin Operators

It is more instructive to consider spin squeezing in terms of new spin operators  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  for which the covariance matrix is diagonal. The new spin operators are related to the original spin operators via

$$\begin{aligned}\hat{J}_x &= \hat{S}_z \\ \hat{J}_y &= \sin \theta_p \hat{S}_x + \cos \theta_p \hat{S}_y \\ \hat{J}_z &= -\cos \theta_p \hat{S}_x + \sin \theta_p \hat{S}_y\end{aligned}\tag{115}$$

corresponding to the transformation in Eq. (57) with Euler angles  $\alpha = -\pi + \theta_p$ ,  $\beta = -\pi/2$  and  $\gamma = -\pi$ .

#### 4.5.3 Bloch Vector and Covariance Matrix

The Bloch vector and covariance matrix for spin operators  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  are given by (see Eqs. (180), (181) in [56] - note that the  $C(\hat{J}_y, \hat{J}_y)$  element is incorrect in Eq. (181))

$$\langle \hat{J}_x \rangle = 0 \quad \langle \hat{J}_y \rangle = 0 \quad \langle \hat{J}_z \rangle = -N \frac{\pi}{8} \tag{116}$$

and

$$\begin{aligned}& \begin{bmatrix} C(\hat{J}_x, \hat{J}_x) & C(\hat{J}_x, \hat{J}_y) & C(\hat{J}_x, \hat{J}_z) \\ C(\hat{J}_y, \hat{J}_x) & C(\hat{J}_y, \hat{J}_y) & C(\hat{J}_y, \hat{J}_z) \\ C(\hat{J}_z, \hat{J}_x) & C(\hat{J}_z, \hat{J}_y) & C(\hat{J}_z, \hat{J}_z) \end{bmatrix} \\ & \doteq \begin{bmatrix} \frac{1}{12}N^2 & 0 & 0 \\ 0 & \frac{1}{4} + \frac{1}{8} \ln N & 0 \\ 0 & 0 & \left(\frac{1}{6} - \frac{\pi^2}{64}\right)N^2 \end{bmatrix} \quad N \gg 1\end{aligned}\tag{117}$$

With  $\langle \Delta \hat{J}_x^2 \rangle = \frac{1}{12}N^2$ ,  $\langle \Delta \hat{J}_y^2 \rangle = \frac{1}{4} + \frac{1}{8} \ln N$  and  $\langle \Delta \hat{J}_z^2 \rangle = \left(\frac{1}{6} - \frac{\pi^2}{64}\right)N^2$  and the only non-zero Bloch vector component being  $\langle \hat{J}_z \rangle = -N \frac{\pi}{8}$  it is easy to see that  $\langle \Delta \hat{J}_x^2 \rangle \langle \Delta \hat{J}_y^2 \rangle \geq \frac{1}{4} |\langle \hat{J}_z \rangle|^2$  as required by the Heisenberg Uncertainty Principle. The principal spin fluctuations in both  $\hat{J}_x$  and  $\hat{J}_z$  are comparable to the length of the Bloch vector and no spin squeezing occurs in either of these components. However, spin squeezing occurs in that  $\hat{J}_y$  is squeezed with respect to  $\hat{J}_x$  -  $\langle \Delta \hat{J}_y^2 \rangle$  only increases as  $\frac{1}{8} \ln N$  whilst  $\frac{1}{2} |\langle \hat{J}_z \rangle|$  increases as  $\frac{\pi}{16}N$  for large  $N$ . Hence the relative phase state satisfies the test in Eq. (95) to demonstrate entanglement for modes  $\hat{c}, \hat{d}$ .

#### 4.5.4 New Modes Operators

To confirm that the relative phase state is in fact an entangled state for modes  $\hat{c}, \hat{d}$  as well as for the original modes  $\hat{a}, \hat{b}$ , we note that the new mode operators

$\hat{c}, \hat{d}$  are given in Eq. (71) with Euler angles  $\alpha = -\pi + \theta_p$ ,  $\beta = -\pi/2$  and  $\gamma = -\pi$ . The old mode operators are given in Eq. (73) and with these Euler angles we have

$$\begin{aligned}\hat{a} &= -\exp(\frac{1}{2}i\theta_p)\frac{1}{\sqrt{2}}(\hat{c}-\hat{d}) \\ \hat{b} &= -\exp(-\frac{1}{2}i\theta_p)\frac{1}{\sqrt{2}}(\hat{c}+\hat{d})\end{aligned}\tag{118}$$

This enables us to write the phase state in terms of new mode operators  $\hat{c}, \hat{d}$  as

$$\begin{aligned}\left|\frac{N}{2}, \theta_p\right\rangle &= \frac{1}{\sqrt{N+1}}\left(\frac{-1}{\sqrt{2}}\right)^N \sum_{k=-N/2}^{N/2} \sum_{r=-N/4+k/2}^{N/4-k/2} \sum_{s=-N/4-k/2}^{N/4+k/2} \\ &\times \frac{1}{\sqrt{(N/2-k)!}} \frac{1}{\sqrt{(N/2+k)!}} (-1)^{N/4-k/2+r} \\ &\times \frac{(N/2-k)!}{(N/4-k/2-r)!(N/4-k/2+r)!} \frac{(N/2+k)!}{(N/4+k/2-s)!(N/4+k/2+s)!} \\ &\times (\hat{c}^\dagger)^{N/2-(r+s)} (\hat{d}^\dagger)^{N/2+(r+s)} |0\rangle\end{aligned}\tag{119}$$

We see that the expression does not depend explicitly on the relative phase  $\theta_p$  when written in terms of the new mode unnormalised Fock states  $(\hat{c}^\dagger)^{N/2-(r+s)} (\hat{d}^\dagger)^{N/2+(r+s)} |0\rangle$ . This pure state is a linear combination of product states of the form  $|N/2-m\rangle_c \otimes |N/2+m\rangle_d$  for various  $m$  - each of which is an  $N$  boson state and an eigenstate for  $\hat{J}_z$  with eigenvalue  $m$ , and therefore is an entangled state for modes  $\hat{c}, \hat{d}$  which is compatible with the global super-selection rule. Note that there cannot just be a single term  $m$  involved, otherwise the variance for  $\hat{J}_z$  would be zero instead of  $\left(\frac{1}{6} - \frac{\pi^2}{64}\right) N^2$ . We will return to the relative phase state again in SubSection 5.1.

## 4.6 Bloch Vector Entanglement Test

We have seen for the general non-entangled states of modes  $\hat{c}$  and  $\hat{d}$  or of modes  $\hat{a}$  and  $\hat{b}$  that

$$\langle \hat{J}_x \rangle = 0 \quad \langle \hat{J}_y \rangle = 0 \tag{120}$$

$$\langle \hat{S}_x \rangle = 0 \quad \langle \hat{S}_y \rangle = 0 \tag{121}$$

From Eqs. (69) and (55) these results are equivalent to

$$\langle \hat{d}\hat{c}^\dagger \rangle = 0 \quad \langle \hat{c}\hat{d}^\dagger \rangle = 0 \tag{122}$$

$$\langle \hat{b}\hat{a}^\dagger \rangle = 0 \quad \langle \hat{a}\hat{b}^\dagger \rangle = 0 \tag{123}$$

Hence we find further *tests* for *entangled states* of modes  $\hat{c}$  and  $\hat{d}$  or of modes  $\hat{a}$  and  $\hat{b}$

$$|\langle \hat{d} \hat{c}^\dagger \rangle|^2 > 0 \quad |\langle \hat{c} \hat{d}^\dagger \rangle|^2 > 0 \quad (124)$$

$$|\langle \hat{b} \hat{a}^\dagger \rangle|^2 > 0 \quad |\langle \hat{a} \hat{b}^\dagger \rangle|^2 > 0 \quad (125)$$

As we will see in Section 5, these tests are particular cases with  $m = n = 1$  of the simpler entanglement test in Eq. (149) that applies for the situation in the present paper where non-entangled states are required to satisfy the superselection rule.

## 5 Other Proposed Tests for Entanglement

There are a number of inequalities involving not only the variances of the spin operators but also other quantities, that have been derived for testing whether a state for a system of identical bosons is entangled. These are *not* always associated with criteria for spin squeezing. Some of these are based on the implicit assumption that the density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$  in the expression for a non-entangled state are *not* required to conform to the super-selection rule that prohibits quantum superpositions of single mode states with differing numbers of bosons. These results are based in effect on a *different criterion* as to what constitutes an *entangled state*, so of course the resulting inequalities will *differ* from those that would apply if the definition of an entangled state is based on the considerations presented here in this paper - which emphasise the requirement that the density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$  should represent physical states for the separate modes and hence satisfy the super-selection rule. Other results are based on forms of the density operator for non-entangled states that do not satisfy the symmetrisation principle. In this Section we examine a number of such entanglement tests and find that some are not valid, though some may be revised as tests for entangled states defined in accord with symmetrisation and super-selection rules.

### 5.1 Hillery et al 2006

#### 5.1.1 Hillery Spin Variance Entanglement Test

One such entanglement test is presented in the paper by Hillery and Zubairy [29] entitled "Entanglement conditions for two-mode states". The paper actually dealt with EM field modes and the super-selection rule was not applied, so density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$  for photon modes allowed for coherences between states with differing photon numbers, and hence the conditions in Eq. (75) did not apply. However, even for the situation of EM field modes where massless photons are involved, it is argued here that the super-selection rule also should be applied. Conditions involving the variances  $\langle \Delta \hat{S}_x \rangle^2, \langle \Delta \hat{S}_y \rangle^2$  can be obtained by applying similar arguments to those in Section 5. It is found that for the original spin operators  $\hat{S}_x, \hat{S}_y, \hat{S}_z$  and modes  $\hat{a}$  and  $\hat{b}$

$$\begin{aligned} \langle \hat{S}_x^2 \rangle_R &= \frac{1}{4} \langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R + \frac{1}{2} \langle \langle \hat{a}^\dagger \hat{a} \rangle_R \langle \hat{b}^\dagger \hat{b} \rangle_R \rangle + \frac{1}{4} \langle \langle (\hat{b}^\dagger)^2 \rangle_R \langle (\hat{a})^2 \rangle_R + \langle \langle \hat{b} \rangle_R \langle \langle \hat{a}^\dagger \rangle^2 \rangle \rangle \\ \langle \hat{S}_y^2 \rangle_R &= \frac{1}{4} \langle \langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R \rangle + \frac{1}{2} \langle \langle \hat{a}^\dagger \hat{a} \rangle_R \langle \hat{b}^\dagger \hat{b} \rangle_R \rangle - \frac{1}{4} \langle \langle (\hat{b}^\dagger)^2 \rangle_R \langle (\hat{a})^2 \rangle_R + \langle \langle \hat{b} \rangle_R \langle \langle \hat{a}^\dagger \rangle^2 \rangle \rangle \end{aligned} \quad (126)$$

where terms such as  $\langle \langle (\hat{b}^\dagger)^2 \rangle_R$  and  $\langle \langle (\hat{a})^2 \rangle_R$  previously shown to be zero have been retained. Note that in [29] the operators  $\hat{S}_x, \hat{S}_y, \hat{S}_z$  constructed from the EM field mode operators as in Eq. (55) would be related to Stokes parameters



Hence

$$\begin{aligned}
& \langle \hat{S}_x^2 \rangle_R + \langle \hat{S}_y^2 \rangle_R \\
&= \frac{1}{2} (\langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R + (\langle \hat{a}^\dagger \hat{a} \rangle_R \langle \hat{b}^\dagger \hat{b} \rangle_R)) \\
&= \frac{1}{2} (\langle \hat{b}^\dagger \hat{b} \rangle_R (\langle \hat{a}^\dagger \hat{a} \rangle_R + 1) + \frac{1}{2} (\langle \hat{a}^\dagger \hat{a} \rangle_R (\langle \hat{b}^\dagger \hat{b} \rangle_R + 1)) \quad (127)
\end{aligned}$$

where the terms  $\langle (\hat{b}^\dagger)^2 \rangle_R, \dots, \langle (\hat{a}^\dagger)^2 \rangle_R$  cancel out. This is the same as before.

However,

$$\begin{aligned}
\langle \hat{S}_x \rangle_R &= \frac{1}{2} (\langle \hat{b}^\dagger \rangle_R \langle \hat{a} \rangle_R + \langle \hat{a}^\dagger \rangle_R \langle \hat{b} \rangle_R) \\
\langle \hat{S}_y \rangle_R &= \frac{1}{2i} (\langle \hat{b}^\dagger \rangle_R \langle \hat{a} \rangle_R - \langle \hat{a}^\dagger \rangle_R \langle \hat{b} \rangle_R) \quad (128)
\end{aligned}$$

is now non-zero, since the previously zero terms have again been retained. Hence

$$\langle \hat{S}_x \rangle_R^2 + \langle \hat{S}_y \rangle_R^2 = \langle \hat{b}^\dagger \rangle_R \langle \hat{b} \rangle_R \langle \hat{a}^\dagger \rangle_R \langle \hat{a} \rangle_R \quad (129)$$

so that we now have

$$\begin{aligned}
& \langle \Delta \hat{S}_x^2 \rangle_R + \langle \Delta \hat{S}_y^2 \rangle_R \\
&= \frac{1}{2} (\langle \hat{b}^\dagger \hat{b} \rangle_R (\langle \hat{a}^\dagger \hat{a} \rangle_R + 1) + \frac{1}{2} (\langle \hat{a}^\dagger \hat{a} \rangle_R (\langle \hat{b}^\dagger \hat{b} \rangle_R + 1) - \langle \hat{b}^\dagger \rangle_R \langle \hat{b} \rangle_R \langle \hat{a} \rangle_R \langle \hat{a}^\dagger \rangle_R \langle \hat{a} \rangle_R) \\
&= \frac{1}{2} (\langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R) + (\langle \hat{b}^\dagger \hat{b} \rangle_R (\langle \hat{a}^\dagger \hat{a} \rangle_R - |\langle \hat{a} \rangle_R|^2 |\langle \hat{b}^\dagger \rangle_R|^2)) \quad (130)
\end{aligned}$$

But from the Schwarz inequality - which is based on  $\langle (\hat{a}^\dagger - \langle \hat{a}^\dagger \rangle)(\hat{a} - \langle \hat{a} \rangle) \rangle \geq 0$  for any state

$$|\langle \hat{a} \rangle_R|^2 \leq \langle \hat{a}^\dagger \hat{a} \rangle_R \quad |\langle \hat{b} \rangle_R|^2 \leq \langle \hat{b}^\dagger \hat{b} \rangle_R \quad (131)$$

so that

$$\langle \Delta \hat{S}_x^2 \rangle_R + \langle \Delta \hat{S}_y^2 \rangle_R \geq \frac{1}{2} (\langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R) \quad (132)$$

and thus from Eq. (78) it follows that for a general non entangled state

$$\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq \sum_R P_R \frac{1}{2} (\langle \hat{n}_b \rangle_R + \langle \hat{n}_a \rangle_R) \quad (133)$$

However, half the expectation value of the number operator is

$$\frac{1}{2} \langle \hat{N} \rangle = \frac{1}{2} \langle \hat{n}_a + \hat{n}_b \rangle = \sum_R P_R \frac{1}{2} (\langle \hat{n}_b \rangle_R + \langle \hat{n}_a \rangle_R) \quad (134)$$

so for a non-entangled state

$$\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} \langle \hat{N} \rangle \quad (135)$$

This inequality for non-entangled states is given in [29] (see Eq. (3)). The above proof was based on a different definition of entangled states to that in this paper.

### 5.1.2 Validity of Hillery Test for Local SSR Compatible Non-Entangled States

However, it turns out that the same inequality is *also* valid when the definition of entangled states is the same as in the present paper. We would then find that  $\langle \hat{S}_x \rangle_R = \langle \hat{S}_y \rangle_R = 0$  and hence

$$\langle \Delta \hat{S}_x^2 \rangle_R + \langle \Delta \hat{S}_y^2 \rangle_R = \frac{1}{2} \left( \langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R \right) + \left( \langle \hat{b}^\dagger \hat{b} \rangle_R \langle \hat{a}^\dagger \hat{a} \rangle_R \right) \quad (136)$$

instead of Eq.(130). Since the term  $\langle \hat{b}^\dagger \hat{b} \rangle_R \langle \hat{a}^\dagger \hat{a} \rangle_R$  is always positive we find after applying Eq. (78) that

$$\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} \langle \hat{N} \rangle \quad (137)$$

which is the same as in Eq. (135). Hence, finding that  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle$  would show that the state was entangled, irrespective of whether or not entanglement is defined in terms of non-physical unentangled states. The Hillery et al [29] *entanglement test*

$$\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle \quad (138)$$

is still used in recent papers, for example [50], [71] which deal with the entanglement of sub-systems each consisting of single modes  $\hat{a}$ ,  $\hat{b}$  for a double well situation (in these papers  $\hat{S}_x \rightarrow \hat{J}_{AB}^X$ ,  $\hat{S}_y \rightarrow -\hat{J}_{AB}^Y$ ,  $\hat{S}_z \rightarrow -\hat{J}_{AB}^Z$ ).

### 5.1.3 Non-Applicable Entanglement Test Involving $|\langle \hat{S}_z \rangle|$

Previously we had found for a general non-entangled state that is based on physically valid density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$

$$\begin{aligned} \langle \Delta \hat{S}_x^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| &\geq 0 \\ \langle \Delta \hat{S}_y^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| &\geq 0 \end{aligned} \quad (139)$$

so that the sum of the variances satisfies the inequality

$$\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle| \quad (140)$$

This is another correct inequality required for a non-entangled state as defined in the present paper. It follows that if only physical states  $\hat{\rho}_R^A, \hat{\rho}_R^B$  are allowed, the related *entanglement test* involving  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle$  would be

$$\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle| \quad (141)$$

For *any* quantum state we have

$$|\langle \hat{S}_z \rangle| = \frac{1}{2} |(\langle \hat{n}_b \rangle - \langle \hat{n}_a \rangle)| \leq \frac{1}{2} (\langle \hat{n}_b \rangle + \langle \hat{n}_a \rangle) = \frac{1}{2} \langle \hat{N} \rangle \quad (142)$$

which means that it is now required that  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle$  be less than a quantity that is *smaller* than in the criterion in (135).

However, it should be noted that *all* states, entangled or otherwise, satisfy the inequality  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle|$  so the inequality in (140) - though true, is of no use in establishing whether a state is entangled in the terms of the meaning of entanglement in the present paper. There are *no* quantum states, entangled or otherwise that satisfy the proposed entanglement test given in Eq. (141). This general result was stated by Hillery et al [29]. To show this we write the Heisenberg uncertainty principle for  $\langle \Delta \hat{S}_x^2 \rangle, \langle \Delta \hat{S}_y^2 \rangle$  as  $\langle \Delta \hat{S}_x^2 \rangle \langle \Delta \hat{S}_y^2 \rangle = \xi \frac{1}{4} |\langle \hat{S}_z \rangle|^2$ , where  $\xi \geq 1$ , then

$$\frac{\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle}{|\langle \hat{S}_z \rangle|} = \frac{1}{2} \left( y + \frac{\xi}{y} \right) = F(y) \quad \text{where } y = \frac{\langle \Delta \hat{S}_x^2 \rangle}{\frac{1}{2} |\langle \hat{S}_z \rangle|} \quad (143)$$

It is straightforward to show that  $F(y) \geq 1$  for all  $\xi, y$ . The minimum value is 1, which occurs for  $\xi = 1$  and  $y = 1$ . Even spin squeezed states with  $\langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle|$  still have  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle|$ , so it is *never* found that  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle|$  and hence this latter inequality *cannot* be used as a test for entanglement.

Fortunately - as we have seen, showing that spin squeezing occurs via *either*  $\langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle|$  *or*  $\langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle|$  is sufficient to establish that the state is an entangled state for modes  $\hat{a}, \hat{b}$ , with analogous results if principle spin operators are considered. Applying the Hillery et al entanglement test in Eq. (138) involving  $\frac{1}{2} \langle \hat{N} \rangle$  is also a valid entanglement test, but is usually *less stringent* than the spin squeezing test involving either  $\langle \Delta \hat{S}_x^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle|$  *or*  $\langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} |\langle \hat{S}_z \rangle|$ . For the Hillery et al entanglement test to be satisfied at least one of  $\langle \Delta \hat{S}_x^2 \rangle$  or  $\langle \Delta \hat{S}_y^2 \rangle$  is required to be less than  $\frac{1}{2} \langle \hat{N} \rangle$ , whereas for the spin squeezing test to apply at least one of  $\langle \Delta \hat{S}_x^2 \rangle$  or  $\langle \Delta \hat{S}_y^2 \rangle$  must be less than  $\frac{1}{2} |\langle \hat{S}_z \rangle|$ . The quantity  $\frac{1}{2} |\langle \hat{S}_z \rangle|$  is likely to be smaller than  $\frac{1}{2} \langle \hat{N} \rangle$  - for example the Bloch vector may lie close to the  $xy$  plane, so a greater degree of reduction in spin fluctuation is needed to satisfy the spin squeezing test for entanglement.

However, this is not always the case as the example of the *relative phase state* discussed in SubSection 4.5 shows. The results in the current SubSection can easily be modified to apply to new spin operators  $\hat{J}_x, \hat{J}_y, \hat{J}_z$ , with entanglement being considered for new modes  $\hat{c}$  and  $\hat{d}$ . The Hillery et al [29] entanglement test then becomes

$$\langle \Delta \hat{J}_x^2 \rangle + \langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle \quad (144)$$

In the case of the relative phase eigenstate we have from Eq. (117) that  $\langle \Delta \hat{J}_x^2 \rangle + \langle \Delta \hat{J}_y^2 \rangle = \frac{1}{12} N^2 + \frac{1}{4} + \frac{1}{8} \ln N \approx \frac{1}{12} N^2$  for large  $N$ . This clearly exceeds  $\frac{1}{2} \langle \hat{N} \rangle = \frac{1}{2} N$ , so the Hillery et al [29] test for entanglement fails. On the other hand, as we have seen in SubSection 4.5  $\langle \Delta \hat{J}_y^2 \rangle < \frac{1}{2} |\langle \hat{J}_z \rangle| \approx \frac{\pi}{16} N$ , so the spin squeezing test is satisfied for this entangled state of modes  $\hat{c}$  and  $\hat{d}$ .

## 5.2 Hillery et al 2009

### 5.2.1 Hillery Strong Correlation Entanglement Test

In a later paper entitled "Detecting entanglement with non-Hermitian operators" Hillery et al [30] apply other inequalities for determining entanglement derived in the earlier paper [29] but now also to systems of massive identical bosons, while still retaining density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$  that contain coherences between states with differing boson numbers. In particular, for a non-entangled state the following family of inequalities - originally derived in [29], is invoked.

$$|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 \leq \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle \quad (145)$$

Thus if  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle$  then the state is entangled.

A particular case for  $n = m = 1$  is the test  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 > \langle \hat{n}_a \hat{n}_b \rangle$  for an entangled state. To put this result in context, for a general quantum state and any operator  $\hat{\Omega}$  we have  $\langle \hat{\Omega}^\dagger \rangle = \langle \hat{\Omega} \rangle^*$  and  $\langle (\hat{\Omega}^\dagger - \langle \hat{\Omega}^\dagger \rangle) (\hat{\Omega} - \langle \hat{\Omega} \rangle) \rangle \geq 0$ , hence leading to the Schwarz inequality  $|\langle \hat{\Omega} \rangle|^2 = |\langle \hat{\Omega}^\dagger \rangle|^2 \leq \langle \hat{\Omega}^\dagger \hat{\Omega} \rangle$ . Taking  $\hat{\Omega} = \hat{a} \hat{b}^\dagger$  leads to the inequality  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 \leq \langle \hat{n}_a (\hat{n}_b + 1) \rangle$ , whilst choosing  $\hat{\Omega} = \hat{b} \hat{a}^\dagger$  leads to the inequality  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 \leq \langle (\hat{n}_a + 1) \hat{n}_b \rangle$  for *all* quantum states. In both cases the right side of the inequality is greater than  $\langle \hat{n}_a \hat{n}_b \rangle$ , so *if* it was found that  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 > \langle \hat{n}_a \hat{n}_b \rangle$  (though of course still  $\leq \langle \hat{n}_a (\hat{n}_b + 1) \rangle$  and  $\leq \langle (\hat{n}_a + 1) \hat{n}_b \rangle$ ) then it could be concluded that the state was entangled. However, as we will see the left side  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2$  actually works out to be zero if physical states for  $\hat{\rho}_R^A, \hat{\rho}_R^B$  are involved in defining non-entangled states, so that for a non-entangled state defined as in the present paper the true inequality

replacing  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 \leq \langle \hat{n}_a \hat{n}_b \rangle$  is just  $0 \leq \langle \hat{n}_a \hat{n}_b \rangle$ , which is trivially true for any quantum state. The test for entanglement requires modification.

The derivation of the general inequality in [29], as in Eq. (145) follows directly from the inequality in Eq. (23) obtained in SubSection 2.5 for a general non-entangled state of sub-systems  $A$  and  $B$ . If we choose  $\hat{\Omega}_A = (\hat{a})^m$  and  $\hat{\Omega}_B = (\hat{b})^n$  then from  $|\langle \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \rangle|^2 \leq \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \otimes \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle$  the result of Hillery et al [29] stated in Eq. (145) immediately follows. The Hillery et al [29] *entanglement test* is that if

$$|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle \quad (146)$$

then it may be concluded that the state is an entangled state for sub-systems  $A$  and  $B$ . Note that the proof of this result did *not* depend on the sub-system density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$  being required to satisfy SSR.

### 5.2.2 Correlation Test for Entanglement for Local SSR Compatible Non-Entangled States

However, for a non-entangled state based on *physical*  $\hat{\rho}_R^A, \hat{\rho}_R^B$  for modes  $\hat{a}$  and  $\hat{b}$  where the SSR is satisfied we actually have

$$\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle = \sum_R P_R \langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle_R = \sum_R P_R \langle (\hat{a})^m \rangle_R \langle (\hat{b}^\dagger)^n \rangle_R = 0 \quad (147)$$

since from Eqs. analogous to (75)  $\langle (\hat{a})^m \rangle_R = \langle (\hat{b}^\dagger)^n \rangle_R = 0$ . Hence for a physical non-entangled state as defined in the present paper the inequality becomes

$$0 \leq \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle \quad (148)$$

which is trivially true and applies for *any* state, entangled or not.

Since  $\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle$  is zero for non-entangled states it follows that it is merely necessary to show that this quantity is non-zero to establish that the state is entangled. Hence an *entanglement test* in the case of sub-systems consisting of single modes  $\hat{a}$  and  $\hat{b}$  becomes

$$|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > 0 \quad (149)$$

for a non-entangled state based on *physical*  $\hat{\rho}_R^A, \hat{\rho}_R^B$ . This is a useful criterion for entanglement in terms the definition of entanglement in the present paper, and is different to that of Hillery et al [29]. The Hillery et al [29] entanglement test  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle$  is *also* a valid test for entanglement and is actually a *more stringent test* than merely showing that  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > 0$ , since the quantity  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2$  is now required to be *larger*. In a paper by He et al [50] (see Section IIIA) the Hillery et al [29] entanglement test  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle$  is applied for the

case where  $A$  and  $B$  each consist of *one mode* localised in each well of a double well potential. This test whilst applicable could be replaced by the more easily satisfied test  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > 0$ . However, as will be seen below in SubSection 5.6, Hillery et al [29] entanglement criterion is needed if the sub-systems each consist of *pairs of modes*, as treated in [72], [50].

### 5.2.3 Examples Applying Correlation Tests for Entanglement

As an example of applying these tests consider the *mixed two mode coherent states* described in SubSection 2.10, whose density operator for the two mode  $\hat{a}$ ,  $\hat{b}$  system is given in Eq. (48). We can now examine the Hillery et al [30] entanglement test in Eq.(146) and the entanglement test in Eq.(149) for the case where  $m = n = 1$ . It is straight-forward to show that

$$\begin{aligned} |\langle \hat{a} \hat{b}^\dagger \rangle|^2 &= |\alpha|^4 \\ \langle (\hat{a}^\dagger \hat{a}) (\hat{b}^\dagger \hat{b}) \rangle &= |\alpha|^4 \end{aligned} \quad (150)$$

so that  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 = \langle (\hat{a}^\dagger \hat{a}) (\hat{b}^\dagger \hat{b}) \rangle$ . A non-entangled state defined in terms of the SSR requirement for the separate modes satisfies  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 = 0$ , whilst for a non-entangled state in which the SSR requirement for separate modes is not specifically required merely satisfies  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 \leq \langle (\hat{a}^\dagger \hat{a}) (\hat{b}^\dagger \hat{b}) \rangle$ . Hence the test for entanglement of modes  $A$ ,  $B$  in the present paper  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 > 0$  is satisfied, whilst the Hillery et al [30] test  $|\langle \hat{a} \hat{b}^\dagger \rangle|^2 > \langle (\hat{a}^\dagger \hat{a}) (\hat{b}^\dagger \hat{b}) \rangle$  is not.

In terms of the definition of non-entangled states in the present paper, the mixture of two mode coherent states given in Eq.(48) is an *entangled state*, not a separable state. However, in terms of the definition of non-entangled states in other papers such as those of Hillery et al [29], [30] the mixture of two mode coherent states would be a *non-entangled state*. It is thus a useful state for providing an example of the different outcomes of definitions where the local SSR is applied or not.

## 5.3 Sorensen et al 2001

### 5.3.1 Sorensen Spin Squeezing Entanglement Test

In a paper entitled "Many-particle entanglement with Bose-Einstein condensates" Sorensen et al [41] consider the implications for spin squeezing for non-entangled states of the form in Eq. (24). As discussed previously, a density operator of this general form is not consistent with the symmetrisation principle - having separate density operators  $\hat{\rho}_R^i$  for specific particles  $i$  in an identical particle system (such as for a BEC) is not compatible with the indistinguishability of such particles. It is modes that are distinguishable, not identical particles,

so the basis for applying their results to systems of identical bosons is flawed. However, they derive an inequality for the spin variance  $\langle \Delta \hat{S}_z^2 \rangle$

$$\langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right) \quad (151)$$

that applies in the case of non-entangled states. Key steps in their derivation are stated in the Appendix to [41], but as the justification of these steps is not obvious for completeness the full derivation is given in Appendix 14 of the present paper. This inequality (151) establishes that if

$$\xi^2 = \frac{\langle \Delta \hat{S}_z^2 \rangle}{\left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right)} < \frac{1}{N} \quad (152)$$

then the state is entangled, so that if the condition for spin squeezing analogous to that in Eq. (64) is satisfied, then entanglement is required if spin squeezing for  $\hat{S}_z$  to occur. Spin squeezing is then a test for entanglement in terms of their definition of an entangled state. Note that the condition (64) requires the Bloch vector to be in the  $xy$  plane and close to the Bloch sphere of radius  $N/2$ .

### 5.3.2 Revising Sorensen Spin Squeezing Entanglement Test - Localised Modes

The work of Sorensen et al really applies only when the individual spins are distinguishable. It is possible however to modify the work of Sorensen et al [41] to apply to a system of identical bosons in accordance with the symmetrisation and super-selection rules if the index  $i$  is *re-interpreted* as specifying different modes, for example modes localised on *optical lattice* sites  $i = 1, 2, \dots, N$ . Details are given in Appendix 15. With two single particle states  $a, b$  available on each site (these could be two different internal atomic states or two distinct spatial modes localised on the site) the modes would then be labelled  $|\phi_{\alpha i}\rangle$  with  $\alpha = a, b$ . The mode orthogonality and completeness relations would then be

$$\begin{aligned} \langle \phi_{\alpha i} | \phi_{\beta j} \rangle &= \delta_{\alpha\beta} \delta_{ij} \\ \sum_{\alpha i} |\phi_{\alpha i}\rangle \langle \phi_{\alpha i}| &= \hat{1} \end{aligned} \quad (153)$$

With the particles now labelled  $K = 1, 2, 3, \dots$  one can define spin operators in first quantization via

$$\begin{aligned} \hat{S}_x &= \sum_K \sum_i (|\phi_{bi}(K)\rangle \langle \phi_{ai}(K)| + |\phi_{ai}(K)\rangle \langle \phi_{bi}(K)|) / 2 \\ \hat{S}_y &= \sum_K \sum_i (|\phi_{bi}(K)\rangle \langle \phi_{ai}(K)| - |\phi_{ai}(K)\rangle \langle \phi_{bi}(K)|) / 2i \\ \hat{S}_z &= \sum_K \sum_i (|\phi_{bi}(K)\rangle \langle \phi_{bi}(K)| - |\phi_{ai}(K)\rangle \langle \phi_{ai}(K)|) / 2 \end{aligned} \quad (154)$$

In second quantization if the annihilation, creation operators for the modes  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  are  $\hat{a}_i, \hat{b}_i$  and  $\hat{a}_i^\dagger, \hat{b}_i^\dagger$  respectively, then the Schwinger spin operators are just

$$\begin{aligned}\hat{S}_x &= \sum_i (\hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i)/2 = \sum_i \hat{S}_x^i \\ \hat{S}_y &= \sum_i (\hat{b}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{b}_i)/2i = \sum_i \hat{S}_y^i \\ \hat{S}_z &= \sum_i (\hat{b}_i^\dagger \hat{b}_i - \hat{a}_i^\dagger \hat{a}_i)/2 = \sum_i \hat{S}_z^i\end{aligned}\quad (155)$$

It is easy to confirm that the overall spin operators  $\hat{S}_\alpha$  and the spin operators  $\hat{S}_\alpha^i$  for the separate *pairs of modes*  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  (or  $\hat{a}_i, \hat{b}_i$  for short) satisfy the same commutation rules as Sorensen et al [41] have for the overall spin operators and those for the separate *particles*. With this modification the non-entangled state in Eq. (24) could be interpreted as being a non-entangled state where the subsystems are actually *pairs of modes*  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  and the density operators  $\hat{\rho}_R^i$  would then refer to a subsystem consisting of these pairs of modes. It is to be noted that entanglement of *pairs* of modes is different to entanglement of *all separate* modes. It is an example of a special kind of *multimode entanglement* - since the modes  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  may themselves be entangled we may have "entanglement of entanglement". In terms of the present paper the density operators  $\hat{\rho}_R^i$  would be restricted by the super-selection rule to statistical mixtures of states with specific total numbers  $N_i$  of bosons in the pair of modes  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$ . In terms of Fock states  $|n_{ai}\rangle, |n_{bi}\rangle$  for this pair of modes the allowed quantum states for the sub-system will be

$$|\Phi_{N_i}\rangle = \sum_{k=0}^{N_i} A_k^{N_i} |k\rangle_{ai} |N_i - k\rangle_{bi} \quad (156)$$

so at this stage the general mixed physical state for the two mode system *could* be

$$\hat{\rho}_R^i = \sum_{N_i=0}^{\infty} \sum_{\Phi} P_{\Phi N_i} \sum_{k=0}^{N_i} \sum_{l=0}^{N_i} A_k^{N_i} (A_l^N)^* |k\rangle_{ai} \langle l|_{ai} \otimes |N_i - k\rangle_{bi} \langle N_i - l|_{bi} \quad (157)$$

This state has no coherences between states of the two mode subsystem with differing total boson number  $N_i$  for the pair of modes. However this is still an entangled states for the two modes  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$ , so the overall state in Eq. (24) is not a non-entangled state if the subsystems were to consist of *all* the distinct modes.

### 5.3.3 Revising Sorensen Spin Squeezing Entanglement Test - Separable State of All Modes

It is possible however to link spin squeezing and entanglement in the case where the sub-systems consist of *all* the distinct modes. To obtain a *fully non-entangled*



state of *all* the modes  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  the density operator  $\hat{\rho}_R^i$  must then be a product of density operators for modes  $|\phi_{ai}\rangle$  and  $|\phi_{bi}\rangle$

$$\hat{\rho}_R^i = \hat{\rho}_R^{a,i} \otimes \hat{\rho}_R^{b,i} \quad (158)$$

giving the full density operator as

$$\hat{\rho} = \sum_R P_R \left( \hat{\rho}_R^{a,1} \otimes \hat{\rho}_R^{b,1} \right) \otimes \left( \hat{\rho}_R^{a,2} \otimes \hat{\rho}_R^{b,2} \right) \otimes \left( \hat{\rho}_R^{a,3} \otimes \hat{\rho}_R^{b,3} \right) \otimes \dots \quad (159)$$

as is required for a general non-entangled state all  $2N$  modes. Furthermore, as previously the density operators for the individual modes must represent possible physical states for such modes, so the super-selection rule for atom number will apply and we have

$$\begin{aligned} \langle (\hat{a}_i)^n \rangle_{a,i} &= \text{Tr}(\hat{\rho}_R^{a,i} (\hat{a}_i)^n) = 0 & \langle (\hat{a}_i^\dagger)^n \rangle_{a,i} &= \text{Tr}(\hat{\rho}_R^{a,i} (\hat{a}_i^\dagger)^n) = 0 \\ \langle (\hat{b}_i)^m \rangle_{b,i} &= \text{Tr}(\hat{\rho}_R^{b,i} (\hat{b}_i)^m) = 0 & \langle (\hat{b}_i^\dagger)^m \rangle_{b,i} &= \text{Tr}(\hat{\rho}_R^{b,i} (\hat{b}_i^\dagger)^m) = 0 \end{aligned} \quad (160)$$

The question is whether this reformulation will lead to a useful inequality for the spin variances such as  $\langle \Delta \hat{S}_x^2 \rangle$ . This issue is dealt with in Appendix 15 and it is found that we can indeed show for the general *fully non-entangled* state (159) that

$$\langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle| \quad (161)$$

This shows that if there is spin squeezing in *either*  $\hat{S}_x$  or  $\hat{S}_y$  then the state must be entangled. Note that this result depends on the general non-entangled state being non-entangled for *all* modes and that the density operator for each mode  $\hat{a}_i$  or  $\hat{b}_i$  being a physical state with no coherences between mode Fock states with differing atom numbers. In terms of the revised interpretation of the density operator to refer to a multi-mode system with modes  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  the statement that spin squeezing for systems of identical massive bosons requires all the modes to be entangled is correct. However superposition states of the form (156) that are consistent with the super-selection rule applying to pure states of a two mode system are precluded, and such states ought to be allowed if entanglement of *pairs* of modes rather than of *separate* modes is to be considered.

#### 5.3.4 Revising Sorensen Spin Squeezing Entanglement Test - Separable State of Pairs of Modes

It is also possible however to link spin squeezing and entanglement in the case where the subsystems consist of *pairs* of modes, but only if *further restrictions* are applied. The general *non-entangled* state of the *pairs* of *modes* would actually be of the form

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes \dots \quad (162)$$

where the  $\hat{\rho}_R^i$  are now of the form given in Eq. (157) and no longer are density operators for the  $i$ th identical particle. Unlike in (160) we now have expectation values  $\langle (\hat{a}_i)^n \rangle_i = \text{Tr}(\hat{\rho}_R^i (\hat{a}_i)^n)$  etc that are non-zero, so considerations of the link between spin squeezing and entanglement - now entanglement of pairs of modes, will be different.

If the density operators  $\hat{\rho}_R^i$  associated with the *pair* of modes  $\hat{a}_i, \hat{b}_i$  are all *restricted* to be associated with *one boson states* then this density operator is of the form

$$\begin{aligned} \hat{\rho}_R^i = & \rho_{aa}^i(|1\rangle_{ia} \langle 1|_{ia} \otimes |0\rangle_{ib} \langle 0|_{ib}) + \rho_{ab}^i(|1\rangle_{ia} \langle 0|_{ia} \otimes |0\rangle_{ib} \langle 1|_{ib}) \\ & + \rho_{ba}^i(|0\rangle_{ia} \langle 1|_{ia} \otimes |1\rangle_{ib} \langle 0|_{ib}) + \rho_{bb}^i(|0\rangle_{ia} \langle 0|_{ia} \otimes |1\rangle_{ib} \langle 1|_{ib}) \end{aligned} \quad (163)$$

where the  $\rho_{ef}^i$  are density matrix elements. With this restriction the pair of modes  $\hat{a}_i, \hat{b}_i$  behave like *distinguishable* two state particles, essentially the case that Sorensen et al [41] implicitly considered. The expectation values for the spin operators  $\hat{S}_x, \hat{S}_y$  and  $\hat{S}_z$  associated with the  $i$ th pair of modes are then

$$\begin{aligned} \langle \hat{S}_x \rangle_R &= \frac{1}{2} (\rho_{ab}^i + \rho_{ba}^i) & \langle \hat{S}_y \rangle_R &= \frac{1}{2i} (\rho_{ab}^i - \rho_{ba}^i) \\ \langle \hat{S}_z \rangle_R &= \frac{1}{2} (\rho_{bb}^i - \rho_{aa}^i) \end{aligned} \quad (164)$$

If in addition Hermitiancy, positivity, unit trace  $\text{Tr}(\hat{\rho}_R^i) = 1$  and  $\text{Tr}(\hat{\rho}_R^i)^2 \leq 1$  are used (see Appendix 14) then we can show that  $\rho_{bb}^i$  and  $\rho_{aa}^i$  are real and positive,  $\rho_{ab}^i = (\rho_{ba}^i)^*$  and  $\rho_{aa}^i \rho_{bb}^i - |\rho_{ab}^i|^2 \geq 0$ . The condition  $\text{Tr}(\hat{\rho}_R^i) = 1$  leads to  $\rho_{aa}^i + \rho_{bb}^i = 1$ , from which  $\text{Tr}(\hat{\rho}_R^i)^2 \leq 1$  follows using the previous positivity results. These results enable the matrix elements in (163) to be parameterised in the form

$$\begin{aligned} \rho_{aa}^i &= \sin^2 \alpha_i & \rho_{bb}^i &= \cos^2 \alpha_i \\ \rho_{ab}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \sin^2 \beta_i \exp(+i\phi_i) & \rho_{ba}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \sin^2 \beta_i \exp(-i\phi_i) \end{aligned} \quad (165)$$

where  $\alpha_i, \beta_i$  and  $\phi_i$  are real. In terms of these quantities we then have

$$\begin{aligned} \langle \hat{S}_x \rangle_R &= \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \cos \phi_i & \langle \hat{S}_y \rangle_R &= \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \sin \phi_i \\ \langle \hat{S}_z \rangle_R &= \frac{1}{2} \cos 2\alpha_i \end{aligned} \quad (166)$$

and then a key inequality

$$\langle \hat{S}_x \rangle_R^2 + \langle \hat{S}_y \rangle_R^2 + \langle \hat{S}_z \rangle_R^2 = \frac{1}{4} - \frac{1}{4} \sin^2 2\alpha_i (1 - \sin^4 \beta_i) \leq \frac{1}{4} \quad (167)$$

follows. This result depends on the density operators  $\hat{\rho}_R^i$  being for one boson states, as in (163). The same steps as in Sorensen et al [41] (see Appendix 14) leads to the result

$$\langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right) \quad (168)$$

for non-entangled *pair* of modes  $\hat{a}_i, \hat{b}_i$ . Thus when the interpretation is changed so that the separate sub-systems are these pairs of modes *and* the sub-systems are in one boson states, it follows that spin squeezing requires entanglement of all the mode pairs.

A similar proof extending the test of Sorensen et al [41] to apply to systems of identical bosons is given by Hyllus et al [44] based on a particle entanglement approach. In their approach bosons in differing external modes (analogous to differing  $i$  here) are treated as distinguishable, and the symmetrization principle is ignored for such bosons.

#### 5.4 Sorensen and Molmer 2001

In a paper entitled "Entanglement and Extreme Spin Squeezing" Sorensen and Molmer [73] first consider the limits imposed by the Heisenberg uncertainty principle on the variance  $\langle \Delta \hat{J}_x^2 \rangle$  considered as a function of  $|\langle \hat{J}_z \rangle|$  for states where the spin operators are chosen such that  $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$ . Note that such spin operators can always be chosen so that the Bloch vector does lie along the  $z$  axis, even if the spin operators are not principal spin operators. Their treatment is based on combining the result from the Schwarz inequality

$$\langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle + \langle \hat{J}_z \rangle^2 \leq J(J+1) \quad (169)$$

where  $J = N/2$ , and the Heisenberg uncertainty principle

$$\langle \Delta \hat{J}_x^2 \rangle \langle \Delta \hat{J}_y^2 \rangle = \xi \frac{1}{4} |\langle \hat{J}_z \rangle|^2 \quad (170)$$

where  $\xi \geq 1$ . In fact two inequalities can be obtained

$$\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} \left\{ \left( J(J+1) - \langle \hat{J}_z \rangle^2 \right) - \sqrt{\left( J(J+1) - \langle \hat{J}_z \rangle^2 \right)^2 - \xi \langle \hat{J}_z \rangle^2} \right\} \quad (171)$$

$$\langle \Delta \hat{J}_x^2 \rangle \leq \frac{1}{2} \left\{ \left( J(J+1) - \langle \hat{J}_z \rangle^2 \right) + \sqrt{\left( J(J+1) - \langle \hat{J}_z \rangle^2 \right)^2 - \xi \langle \hat{J}_z \rangle^2} \right\} \quad (172)$$

which restricts the region in a  $\langle \Delta \hat{J}_x^2 \rangle$  versus  $|\langle \hat{J}_z \rangle|$  plane that applies for states that are consistent with the Heisenberg uncertainty principle. The first

of these two inequalities is given as Eq. (3) in [73]. For states in which  $\hat{J}_x$  is squeezed relative to  $\hat{J}_y$  the points in the  $\langle \Delta \hat{J}_x^2 \rangle$  versus  $|\langle \hat{J}_z \rangle|$  plane must also satisfy

$$\langle \Delta \hat{J}_x^2 \rangle \leq \frac{1}{2} |\langle \hat{J}_z \rangle| \quad (173)$$

Note that as  $\hat{J}_z$  is a spin angular momentum component we always have  $|\langle \hat{J}_z \rangle| \leq J$ , which places an overall restriction on  $|\langle \hat{J}_z \rangle|$ . However, for  $\xi > 1$  there are values of  $|\langle \hat{J}_z \rangle|$  which are excluded via the Heisenberg uncertainty principle, since the quantity  $\left( J(J+1) - \langle \hat{J}_z \rangle^2 \right)^2 - \xi \langle \hat{J}_z \rangle^2$  then becomes negative. This effect is seen in Figure 4.

The question is: Is it possible to find values for  $\langle \Delta \hat{J}_x^2 \rangle$  and  $|\langle \hat{J}_z \rangle|$  in which all three inequalities are satisfied? The answer is yes. Results showing the regions in the  $\langle \Delta \hat{J}_x^2 \rangle$  versus  $|\langle \hat{J}_z \rangle|$  plane corresponding to the three inequalities are shown in Figures 2 and 3 for the cases where  $J = 1000$  and with  $\xi = 1.0$  and  $\xi = 10.0$  respectively. The quantities for which the regions are shown are the scaled variance and mean  $\langle \Delta \hat{J}_x^2 \rangle / J$  and  $|\langle \hat{J}_z \rangle| / J$ , with  $\langle \Delta \hat{J}_x^2 \rangle$  given as a function of  $|\langle \hat{J}_z \rangle|$  via (171), (172) and (173). The spin squeezing region is always consistent with the second Heisenberg inequality (172) and for large  $J = 1000$  there is a large region of overlap with the first inequality (171). For small  $J$  and large  $\xi$  the region of overlap becomes much smaller, as the result in Figure 4 for  $J = 1$  and with  $\xi = 10.0$  shows. As the derivation of the Heisenberg principle inequalities is not obvious, this is set out in Appendix.16.

Sorensen and Molmer [73] also determine the minimum for  $\langle \Delta \hat{J}_x^2 \rangle = \langle \hat{J}_x^2 \rangle$  as a function of  $|\langle \hat{J}_z \rangle|$  for various choices of  $J$ , subject to the constraints  $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$ . The results show again that there is a region in the  $\langle \Delta \hat{J}_x^2 \rangle$  versus  $|\langle \hat{J}_z \rangle|$  plane which is compatible with spin squeezing.

So although these considerations show that the Heisenberg uncertainty principle does not rule out spin squeezing, nothing is determined about whether the spin squeezed states are entangled states for modes  $\hat{c}$ ,  $\hat{d}$ , where the  $\hat{J}_\alpha$  are given as in Eq. (69). The discussion in [73] regarding entanglement is based on the physically incorrect density operator for non-entangled states of identical particles in Eq. (24), discussed in the previous section.

## 5.5 Duan et al 2000

A further inequality aimed at providing a signature for entanglement is set out in the papers by Duan et al [74], Toth et al [75]. For simplicity we only set out the case for which  $a = 1$  in the former paper. This inequality involves position

and momentum like Hermitian operators defined by

$$\begin{aligned}\hat{x}_A &= \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger) & \hat{p}_A &= \frac{1}{\sqrt{2}i}(\hat{a} - \hat{a}^\dagger) \\ \hat{x}_B &= \frac{1}{\sqrt{2}}(\hat{b} + \hat{b}^\dagger) & \hat{p}_B &= \frac{1}{\sqrt{2}i}(\hat{b} - \hat{b}^\dagger)\end{aligned}\quad (174)$$

These are essentially *quadrature operators* and satisfy commutation rules  $[\hat{x}_A, \hat{p}_A] = [\hat{x}_B, \hat{p}_B] = i$  similar to those for position and momentum. An inequality is obtained for a general two mode non-entangled state involving the variances for the commuting observables  $\hat{x}_A + \hat{x}_B$  and  $\hat{p}_A - \hat{p}_B$

$$\langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle \geq 2 \quad (175)$$

which could be used to establish a *quadrature variance test* for entangled states of the mode  $A$  and mode  $B$  sub-systems, so that if

$$\langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle < 2 \quad (176)$$

then the modes are entangled. Such states are possible - consider for example any simultaneous eigenstate of the commuting observables  $\hat{x}_A + \hat{x}_B$  and  $\hat{p}_A - \hat{p}_B$ . For such a state  $\langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle$  and  $\langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle$  are both zero, so the simultaneous eigenstates are entangled states of modes  $A, B$ .

To confirm whether the inequality (175) applies for non-entangled states (101) in which the sub-system states  $\hat{\rho}_R^A, \hat{\rho}_R^B$  are physical, the general variance result in Eq. (78) plus the factorisations  $\langle \hat{x}_A \hat{x}_B \rangle_R = \langle \hat{x}_A \rangle_R \langle \hat{x}_B \rangle_R$  and  $\langle \hat{p}_A \hat{p}_B \rangle_R = \langle \hat{p}_A \rangle_R \langle \hat{p}_B \rangle_R$  are first used to show that

$$\begin{aligned}& \langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle \\ & \geq \sum_R P_R \left( \langle \hat{x}_A^2 \rangle_R - \langle \hat{x}_A \rangle_R^2 + \langle \hat{x}_B^2 \rangle_R - \langle \hat{x}_B \rangle_R^2 + \langle \hat{p}_A^2 \rangle_R - \langle \hat{p}_A \rangle_R^2 + \langle \hat{p}_B^2 \rangle_R - \langle \hat{p}_B \rangle_R^2 \right)\end{aligned}\quad (177)$$

For sub-system states  $\hat{\rho}_R^A, \hat{\rho}_R^B$  that are physical we have in addition  $\langle \hat{x}_A \rangle_R = \langle \hat{x}_B \rangle_R = \langle \hat{p}_A \rangle_R = \langle \hat{p}_B \rangle_R = 0$ . Also using  $\langle \hat{a}^2 \rangle_R = \langle (\hat{a}^\dagger)^2 \rangle_R = \langle \hat{b}^2 \rangle_R = \langle (\hat{b}^\dagger)^2 \rangle_R = 0$  for physical states we find for the remaining terms in Eq.(177) that

$$\begin{aligned}\langle \hat{x}_A^2 \rangle_R &= \frac{1}{2} (\langle \hat{a}^2 \rangle_R + \langle (\hat{a}^\dagger)^2 \rangle_R + 1 + 2 \langle \hat{a}^\dagger \hat{a} \rangle_R) \geq \frac{1}{2} \\ \langle \hat{x}_B^2 \rangle_R &= \frac{1}{2} (\langle \hat{b}^2 \rangle_R + \langle (\hat{b}^\dagger)^2 \rangle_R + 1 + 2 \langle \hat{b}^\dagger \hat{b} \rangle_R) \geq \frac{1}{2} \\ \langle \hat{p}_A^2 \rangle_R &= -\frac{1}{2} (\langle \hat{a}^2 \rangle_R + \langle (\hat{a}^\dagger)^2 \rangle_R - 1 - 2 \langle \hat{a}^\dagger \hat{a} \rangle_R) \geq \frac{1}{2} \\ \langle \hat{p}_B^2 \rangle_R &= -\frac{1}{2} (\langle \hat{b}^2 \rangle_R + \langle (\hat{b}^\dagger)^2 \rangle_R - 1 - 2 \langle \hat{b}^\dagger \hat{b} \rangle_R) \geq \frac{1}{2}\end{aligned}\quad (178)$$

Substituting these results into Eq.(177) establishes the validity of (175) for non-entangled states in which the  $\hat{\rho}_R^A, \hat{\rho}_R^B$  are physical sub-system states. As there are entangled states that violate the inequality (175), this inequality is valid for determining whether a state is entangled.

## 5.6 He et al 2012

In two papers dealing with EPR entanglement He et al [72], [50] a *four mode* system associated with a double well potential is considered. In the left well *A* there are two localised modes with annihilation operators  $\hat{a}_1, \hat{a}_2$  and in the right well *B* there are two localised modes with annihilation operators  $\hat{b}_1, \hat{b}_2$ . The modes in each well could be associated with different internal states or they could be associated with different spatial modes of the same internal state. This four mode system provides for the possibility of entanglement of *two sub-systems* each consisting of *pairs of modes*. With four modes there are three different choices of such sub-systems but perhaps the most interesting from the point of view of entanglement of spatially separated modes - and hence implications for EPR entanglement - would be to have the two *left well modes*  $\hat{a}_1, \hat{a}_2$  as sub-system *A* and the two *right well modes*  $\hat{b}_1, \hat{b}_2$  as sub-system *B*. Consistent with the requirement that the sub-system density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$  conform to the symmetrisation principle and the super-selection rule, these density operators may now be of the form given in Eq. (47). Hence as discussed in Sub-System 2.12, when considering *non-entangled* states for the sub-systems *A* and *B* we now have as in Eq. (54)

$$\begin{aligned} \langle (\hat{a}_i)^n \rangle_A &= \text{Tr}(\hat{\rho}_R^A (\hat{a}_i)^n) \neq 0 & \langle (\hat{a}_i^\dagger)^n \rangle_A &= \text{Tr}(\hat{\rho}_R^A (\hat{a}_i^\dagger)^n) \neq 0 \\ \langle (\hat{b}_j)^m \rangle_B &= \text{Tr}(\hat{\rho}_R^B (\hat{b}_j)^m) \neq 0 & \langle (\hat{b}_j^\dagger)^m \rangle_B &= \text{Tr}(\hat{\rho}_R^B (\hat{b}_j^\dagger)^m) \neq 0 \end{aligned} \quad (179)$$

in general. Hence in this case where the sub-systems are *pairs* of modes the entanglement test in Eq. (149) for sub-systems consisting of *single* modes cannot be applied.

### 5.6.1 Correlation Tests for Entanglement

However, the inequalities derived by Hillery et al [30] (see SubSection 5.2)

$$|\langle (\hat{a}_i)^m (\hat{b}_j^\dagger)^n \rangle|^2 \leq \langle (\hat{a}_i^\dagger)^m (\hat{a}_i)^m (\hat{b}_j^\dagger)^n (\hat{b}_j)^n \rangle \quad (180)$$

that apply for two non-entangled sub-systems *A* and *B* can now be usefully applied, since in this case the quantities  $\langle (\hat{a}_i)^m (\hat{b}_j^\dagger)^n \rangle$  are in general no longer zero. Thus there is an *entanglement test* for two sub-systems consisting of *pairs of modes*. If

$$\begin{aligned} |\langle (\hat{a}_i)^m (\hat{b}_j^\dagger)^n \rangle|^2 &> \langle (\hat{a}_i^\dagger)^m (\hat{a}_i)^m (\hat{b}_j^\dagger)^n (\hat{b}_j)^n \rangle \\ \text{for any of } i, j &= 1, 2 \end{aligned} \quad (181)$$

then the quantum state for two sub-systems  $A$  and  $B$  - *each* consisting of *two modes* localised in each well - is entangled.

### 5.6.2 Spin Squeezing Tests for Entanglement

There are numerous choices for defining spin operators but the most useful would be the *local spin operators* for each well [50] defined by

$$\begin{aligned}\hat{S}_x^A &= (\hat{a}_2^\dagger \hat{a}_1 + \hat{a}_1^\dagger \hat{a}_2)/2 & \hat{S}_y^A &= (\hat{a}_2^\dagger \hat{a}_1 - \hat{a}_1^\dagger \hat{a}_2)/2i & \hat{S}_z^A &= (\hat{a}_2^\dagger \hat{a}_2 - \hat{a}_1^\dagger \hat{a}_1)/2 \\ \hat{S}_x^B &= (\hat{b}_2^\dagger \hat{b}_1 + \hat{b}_1^\dagger \hat{b}_2)/2 & \hat{S}_y^B &= (\hat{b}_2^\dagger \hat{b}_1 - \hat{b}_1^\dagger \hat{b}_2)/2i & \hat{S}_z^B &= (\hat{b}_2^\dagger \hat{b}_2 - \hat{b}_1^\dagger \hat{b}_1)/2\end{aligned}\quad (182)$$

These satisfy the usual angular momentum commutation rules and those of the different wells commute. The squares of the local vector spin operators are related to the total number operators  $\hat{N}_A = \hat{a}_2^\dagger \hat{a}_2 + \hat{a}_1^\dagger \hat{a}_1$  and  $\hat{N}_B = \hat{b}_2^\dagger \hat{b}_2 + \hat{b}_1^\dagger \hat{b}_1$  as  $\sum_{\alpha} (\hat{S}_{\alpha}^A)^2 = (\hat{N}_A/2)(\hat{N}_A/2 + 1)$  and  $\sum_{\alpha} (\hat{S}_{\alpha}^B)^2 = (\hat{N}_B/2)(\hat{N}_B/2 + 1)$ .

For the local spin operators we have in general

$$\langle \hat{S}_{\alpha}^A \rangle_A = \text{Tr}(\hat{\rho}_R^A \hat{S}_{\alpha}^A) \neq 0 \quad \langle \hat{S}_{\alpha}^B \rangle_B = \text{Tr}(\hat{\rho}_R^B \hat{S}_{\alpha}^B) \neq 0 \quad (183)$$

since the pair of modes  $\hat{a}_1, \hat{a}_2$  and/or  $\hat{b}_1, \hat{b}_2$  may now be of the form given in Eq. (47).

In SubSection 2.5 it was shown that  $|\langle \hat{\Omega}_A^\dagger \hat{\Omega}_B \rangle|^2 \leq \langle \hat{\Omega}_A^\dagger \hat{\Omega}_A \hat{\Omega}_B^\dagger \hat{\Omega}_B \rangle$  for a non-entangled state, so with  $\hat{\Omega}_A = \hat{S}_-^A = \hat{S}_x^A - i\hat{S}_y^A$  and  $\hat{\Omega}_B = \hat{S}_-^B = \hat{S}_x^B - i\hat{S}_y^B = (\hat{S}_+^B)^\dagger$  to give

$$|\langle \hat{S}_+^A \hat{S}_-^B \rangle|^2 \leq \langle \hat{S}_+^A \hat{S}_-^A \hat{S}_+^B \hat{S}_-^B \rangle \quad (184)$$

for a non-entangled state of sub-systems  $A$  and  $B$ . For the non-entangled state of these two sub-systems we have

$$\langle \hat{S}_+^A \hat{S}_-^B \rangle = \sum_R P_R \langle \hat{S}_+^A \rangle_A^R \langle \hat{S}_-^B \rangle_B^R \quad (185)$$

which in general is non-zero from Eq.(183).

Hence a valid *entanglement test* involving *spin operators* for sub-systems  $A$  and  $B$  - *each* consisting of *two modes* localised in each well exists, and is if

$$|\langle \hat{S}_+^A \hat{S}_-^B \rangle|^2 > \langle \hat{S}_+^A \hat{S}_-^A \hat{S}_+^B \hat{S}_-^B \rangle \quad (186)$$

then the two sub-systems are entangled. A similar conclusion is stated in [50]. This test for entanglement involves the local spin operators, though it is not then the same as spin squeezing criteria. It is referred to as *spin entanglement*.

## 6 Experiments on Spin Squeezing

There are several papers [76], [77], [78] which contain the results of measuring the spin squeezing parameter analogous to the expression in Eq. (65) and showing that spin squeezing occurs. The presence of entanglement is then inferred by reference to theoretical papers such as [41] that show that spin squeezing only occurs for entangled states - it is an entanglement *witness*. As no independent *measures* of entanglement (however defined) are presented, nor are other independent tests for entanglement carried out, it cannot be said that these paper shows *experimentally* that spin squeezing requires entanglement. In [78] the emphasis is on showing how the spin squeezing can be generated via the non-linear terms in the Josephson Hamiltonian.



## 7 Discussion and Summary of Key Results

This paper is mainly concerned with two mode entanglement for systems of identical bosons and the relationship to spin squeezing. These bosons may be atoms or molecules as in cold quantum gases or may be photons as in quantum optics. The analysis applies to both though detailed arguments are often framed for the bosonic atom case.

A careful analysis is first given regarding the proper definition of a non-entangled state for systems of identical particles, and hence by implication the proper definition of an entangled state. Noting that entanglement is meaningless until the subsystems being entangled are specified, it is pointed out that whereas it is not possible to distinguish identical particles and hence the individual particles are not legitimate sub-systems, the same is not the case for the single particle states or modes, so the *modes* are then the the rightful *sub-systems* to be considered as being entangled or not. In this approach where the sub-systems are modes, situations where there are differing numbers of identical particles are treated as different physical states, not as differing physical systems, and the *symmetrisation principle* required of physical states for identical particle systems will be satisfied by using Fock states to describe the states.

Furthermore, it is argued that the overall physical states should conform to the *superselection rule* that excludes quantum superposition states of the form (26) as physical states for systems of identical particles - massive or otherwise. Although the justification of the SSR in terms of observers and their *reference frames* formulated by other authors has also been presented for completeness, a number of fairly *straightforward reasons* were given for why it is appropriate to apply this superselection rule, which may be summarised as: 1. No way is known for creating such states. 2 No way is known for measuring all the properties of such states, even if they existed. 3. There is no need to invoke the existence of such states in order to understand coherence and interference effects. 4. The stability of such states against decoherence processes may not be great, so even if they could be created they could rapidly change to other states. The last reason is of lesser importance. Invoking the physical existence of states that as far as we know cannot be made or measured, and for which there are no known physical effects that require their presence seems a rather unnecessary feature to add to the non-relativistic quantum physics of many body systems, and considerations based on the general principle of simplicity (Occam's razor) would suggest not doing this until a clear physical justification for including them is found. As two mode fermionic systems are restricted to states with at most two fermions, the focus of the paper is then on bosonic systems, where large numbers of bosons can occupy two mode systems.

However, although there is related work involving local particle number super-selection rules, *this paper differs* from a number of others by *extending* the *super-selection rule* to also apply to the density operators  $\hat{\rho}_R^A$ ,  $\hat{\rho}_R^B$ , .. for the *mode sub-systems*  $A$ ,  $B$ , .that occur in the definition (1) of a *general non-entangled* state for systems of identical particles. Hence it follows that the definition of *entangled states* will differ in this paper from that which would

apply if density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , allowed for coherent superpositions of number states within each mode. In fact more states are regarded as entangled in terms of the definition in the present paper. Indeed, if *further restrictions* are placed on the sub-system density operators - such as requiring them to specify a fixed number of bosons - the set of entangled states is further enlarged. The *simple justification* for our viewpoint on applying the *local particle number super-selection rule* has three aspects. Firstly, since experimental arrangements in which only one bosonic mode is involved can be created, the same reasons (see last paragraph) justify applying the super-selection rule to this mode system as applied for the system as a whole. Secondly, measurements can be carried out on the separate modes, and the joint probability for the outcomes of these measurements determined. For a non-entangled state the joint probability (4) for these measurements depends on all the density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , .. for the mode sub-systems as well as the probability  $P_R$  for the product state  $\hat{\rho}_R^A \otimes \hat{\rho}_R^B$  ..occurring when the general mixed non-entangled state is prepared, which can be accomplished by local preparations and classical communication. For the non-entangled state the form of the joint probability  $P_{AB..}(i, j, ..)$  for measurements on all the sub-systems is given by the products of the individual sub-system probabilities  $P_A^R(i) = Tr(\hat{\Pi}_i^A \hat{\rho}_R^A)$ , etc that measurements on the sub-systems  $A, B$ , ..yield the outcomes  $\lambda_i^A$  etc when the sub-systems are in states  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , .., the overall products being weighted by the probability  $P_R$  that a particular product state is prepared. If  $\hat{\rho}_R^A, \hat{\rho}_R^B$  did not represent physical states then the interpretation of the joint probability as this statistical average would be unphysical. Thirdly, attempts to allow the density operators  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , .. for the mode sub-systems to violate the super-selection rule provided that the reduced density operators  $\hat{\rho}_A, \hat{\rho}_B$  for the separate modes are consistent with it are shown not to be possible in general.

As well as the above justifications for applying the super-selection rule to both the overall multi-mode state for systems of identical particles and the separate sub-system states in the definition of non-entangled states, a more sophisticated justification based on considering SSR to be the consequence of describing the quantum state by an observer (Charlie) whose phase reference is unknown has also been presented in detail in Appendix 11 for completeness. For the sub-systems *local reference frames* are involved. The SSR is seen as a special case of a general SSR which forbids quantum states from exhibiting coherences between states associated with *irreducible representations* of the transformation group that relates reference frames, and which may be the *symmetry group* for the system.

The present paper then defines spin squeezing for two mode systems and discusses the desirability of defining *spin squeezing* in terms of the *principal spin operators*  $\hat{J}_x, \hat{J}_y, \hat{J}_z$  for which the *covariance matrix* is diagonal, rather than via the original spin operators  $\hat{S}_x, \hat{S}_y, \hat{S}_z$  defined in terms of the original mode annihilation and creation operators  $\hat{a}, \hat{b}$  and  $\hat{a}^\dagger, \hat{b}^\dagger$  and for which the covariance matrix is non-diagonal in general. It is seen that the two sets of spin operators are related via a rotation operator and the principal spin operators are given

in terms of *new mode operators*  $\hat{c}, \hat{d}$  and  $\hat{c}^\dagger, \hat{d}^\dagger$ , with  $\hat{c}, \hat{d}$  obtained as linear combinations of the original mode operators  $\hat{a}, \hat{b}$  and hence defining two new modes.

The immediate consequence for the case of two mode systems of identical bosons of the present approach to defining entangled states is that spin squeezing in *any* of the principle spin operators  $\hat{J}_x, \hat{J}_y$  or  $\hat{J}_z$  *requires* entanglement of the new modes  $\hat{c}, \hat{d}$ . Similarly, spin squeezing in *any* of the original spin operators  $\hat{S}_x, \hat{S}_y$  or  $\hat{S}_z$  requires entanglement of the original modes  $\hat{a}, \hat{b}$ . A typical test for entanglement is  $\langle \Delta \hat{S}_x^2 \rangle < |\langle \hat{S}_z \rangle|/2$  or  $\langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle|/2$ . It is noted that though spin squeezing requires entanglement, the opposite is not the case and the *NOON* state provides an example of an entangled physical state that is not spin squeezed. Also, the *binomial state* provides an example of a state that is entangled and spin squeezed for one choice of mode sub-systems may be non-entangled and not spin squeezed for another choice. The *relative phase state* provides an example that is entangled for new modes  $\hat{c}, \hat{d}$  and is highly spin squeezed in  $\hat{J}_y$  and very unsqueezed in  $\hat{J}_x$ . The connection between spin squeezing and entanglement is regarded as well-known, but up to now only proofs based on non-entangled states that either disregard the symmetrization principle or the sub-system super-selection rules exist, placing the connection between spin squeezing and entanglement on a somewhat shaky basis. On the other hand, the proof given here is based on a definition of non-entangled (and hence entangled) states that is compatible with both these requirements.

There are several papers that obtain *different tests* for whether a state is entangled from those involving spin squeezing that are obtained in this paper, the proofs often being based on a definition of non-entangled states that ignores symmetrization or SSR. Hillery et al [29] obtain criteria of this type, such as the entanglement test  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < \frac{1}{2} \langle \hat{N} \rangle$ . This test is also valid if the non-entangled state definition is consistent with the SSR, but is different to the test  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle|$  suggested by the requirement that  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle|$  for non-entangled states - since both  $\langle \Delta \hat{S}_x^2 \rangle \geq |\langle \hat{S}_z \rangle|/2$  and  $\langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle|/2$ . The latter inequality is of no use since  $\langle \Delta \hat{S}_x^2 \rangle + \langle \Delta \hat{S}_y^2 \rangle \geq |\langle \hat{S}_z \rangle|$  for all states. However as previously noted, showing that either  $\langle \Delta \hat{S}_x^2 \rangle < |\langle \hat{S}_z \rangle|/2$  or  $\langle \Delta \hat{S}_y^2 \rangle < |\langle \hat{S}_z \rangle|/2$  - or the analogous tests for other pairs of spin operators - already provides a test for the entanglement of the original modes  $\hat{a}, \hat{b}$ . This test is a different test for entanglement than that of Hillery et al [29]. The case of the *relative phase eigenstate* is an example of an entangled state in which the spin squeezing test for entanglement *succeeds* whereas that of Hillery et al [29] *fails*. Other inequalities found by Hillery et al [30] for non-entangled states which also do not depend on whether non-entangled states satisfy the super-selection rule include  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 \leq \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle$ , giving another valid test

$|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > \langle (\hat{a}^\dagger)^m (\hat{a})^m (\hat{b}^\dagger)^n (\hat{b})^n \rangle$  for an entangled state. However, with entanglement defined as in the present paper we have  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 = 0$  for a non-entangled state, so an entanglement test in the form  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2 > 0$  immediately follows. This test is less stringent than that of Hillery et al [30], as  $|\langle (\hat{a})^m (\hat{b}^\dagger)^n \rangle|^2$  is then required to be larger. Sorensen et al [41] show that spin squeezing is a test for a state being entangled, but define non-entangled states for identical particle systems (such as BECs) in a form that is *inconsistent* with the symmetrisation principle - the sub-systems being regarded as individual identical particles. However, the treatment of Sorensen et al [41] can be modified to apply to a system of identical bosons if the particle index  $i$  is *re-interpreted* as specifying different modes, for example modes localised on optical lattice sites  $i = 1, 2, \dots, N$ . With two single particle states  $|\phi_{ai}\rangle, |\phi_{bi}\rangle$  with annihilation operators  $a_i, b_i$  available on each site, there would then be  $2N$  modes involved, but spin operators can still be defined. If the definitions of non-entangled and entangled states in the present paper are applied, it can be shown that spin squeezing in either of the spin operators  $\hat{S}_x$  or  $\hat{S}_y$  requires entanglement of *all* the original modes  $\hat{a}_i, \hat{b}_i$ . Alternatively, if the sub-systems are *pairs* of modes  $\hat{a}_i, \hat{b}_i$  and the sub-system density operators  $\hat{\rho}_R^i$  were restricted to states with exactly *one boson*, then it can be shown that spin squeezing in  $\hat{S}_z$  requires entanglement of all the pairs of modes. With this restriction the pair of modes  $\hat{a}_i, \hat{b}_i$  behave like *distinguishable* two state particles, which was essentially the case that Sorensen et al [41] implicitly considered. This type of entanglement is a multi-mode entanglement of a special type - since the modes  $\hat{a}_i, \hat{b}_i$  may themselves be entangled there is an "entanglement of entanglement". So with either of these key revisions, the work of Sorensen et al [41] could be said to show that spin squeezing requires entanglement. Sorensen and Molmer [73] have deduced an inequality involving  $\langle \Delta \hat{J}_x^2 \rangle$  and  $|\langle \hat{J}_z \rangle|$  for states where  $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$  based on just the Heisenberg uncertainty principle. This is useful in terms of confirming that states do exist that are spin squeezed still conform to this principle. Duan et al [74], Toth et al [75] devise a test for entanglement based on the sum of the quadrature variances  $\langle \Delta(\hat{x}_A + \hat{x}_B)^2 \rangle + \langle \Delta(\hat{p}_A - \hat{p}_B)^2 \rangle$ , which involve quadrature components  $\hat{x}_A, \hat{p}_A, \hat{x}_B, \hat{p}_B$  constructed from the original mode annihilation, creation operators for modes  $A, B$ . Their conclusion that if the sum is less than 2 then the state is entangled is valid both for the present definition of entanglement and for that in which the application of the super-selection rule is ignored. He et al [72], [50] consider a *four mode* system, with two modes localised in each well of a double well potential. If the two sub-systems  $A$  and  $B$  each consist of two modes - with  $\hat{a}_1, \hat{a}_2$  as sub-system  $A$  and  $\hat{b}_1, \hat{b}_2$  as sub-system  $B$ , then tests of entanglement of the two sub-systems of the Hillery [30] type  $|\langle (\hat{a}_i)^\dagger (\hat{b}_j) \rangle|^2 > \langle (\hat{a}_i^\dagger)^m (\hat{a}_i)^m (\hat{b}_j^\dagger)^n (\hat{b}_j)^n \rangle$  for any  $i, j = 1, 2$  or involving local spin operators  $|\langle \hat{S}_+^A \hat{S}_-^B \rangle|^2 > \langle \hat{S}_+^A \hat{S}_-^A \hat{S}_+^B \hat{S}_-^B \rangle$  apply.

Overall then, all of the *entanglement tests* (spin squeezing and other) in

the other papers discussed here are *still valid* when reconsidered in accord with the definition of entanglement based on the symmetrisation and super-selection rules, though in one case Sorensen et al [41] a re-definition of the sub-systems is required to satisfy the symmetrization principle. However, *further* tests for entanglement are obtained in the present paper based on non-entangled states that are consistent with the symmetrization and super-selection rules. In some cases they are less stringent - the correlation test in Eq.(149) being easier to satisfy than that of Hillery et al [30] in Eq. (146). They are certainly *different* to others previously discovered.

At present, experiments demonstrating spin squeezing do not show experimentally whether spin squeezing requires entanglement, however defined, since no results for entanglement measures are presented, nor are other independent tests for entanglement carried out.

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## 9 Appendix 1 - Inequalities

### 9.1 Integral Inequality

If  $C(\lambda)$  is a real, positive function of  $\lambda$  and  $P(\lambda)$  is another real, positive function such that  $\int d\lambda P(\lambda) = 1$  then we can show that

$$\int d\lambda P(\lambda) C(\lambda) \geq \left( \int d\lambda P(\lambda) \sqrt{C(\lambda)} \right)^2 \quad (187)$$

To show this write  $y = \int d\lambda P(\lambda) C(\lambda)$ . Then

$$\begin{aligned} y &= \int d\mu P(\mu) \int d\lambda P(\lambda) C(\lambda) \\ &= \int \int d\lambda d\mu P(\mu) P(\lambda) C(\lambda) \\ &= \int d\lambda P(\lambda)^2 C(\lambda) + \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\mu) P(\lambda) C(\lambda) \end{aligned} \quad (188)$$

Also, write  $z = \left( \int d\lambda P(\lambda) \sqrt{C(\lambda)} \right)^2$ . Then

$$\begin{aligned} z &= \int d\mu P(\mu) \sqrt{C(\mu)} \int d\lambda P(\lambda) \sqrt{C(\lambda)} \\ &= \int \int d\lambda d\mu P(\mu) P(\lambda) \sqrt{C(\mu)} \sqrt{C(\lambda)} \\ &= \int d\lambda P(\lambda)^2 C(\lambda) + \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\mu) P(\lambda) \sqrt{C(\mu)} \sqrt{C(\lambda)} \end{aligned} \quad (189)$$

so that

$$\begin{aligned} y - z &= \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\mu) P(\lambda) \left( C(\lambda) - \sqrt{C(\mu)} \sqrt{C(\lambda)} \right) \\ &= \frac{1}{2} \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\mu) P(\lambda) \left( C(\lambda) + C(\mu) - 2\sqrt{C(\mu)} \sqrt{C(\lambda)} \right) \\ &= \frac{1}{2} \int \int d\lambda d\mu (1 - \delta(\lambda - \mu)) P(\mu) P(\lambda) \left( \sqrt{C(\lambda)} - \sqrt{C(\mu)} \right)^2 \\ &\geq 0 \end{aligned} \quad (190)$$

which proves the result.

### 9.2 Sum Inequality

If  $C_R$  is a real, positive quantity for various  $R$  and  $P_R$  is another real, positive quantity such that  $\sum_R P_R = 1$  then we can show that

$$\sum_R P_R C_R \geq \left( \sum_R P_R \sqrt{C_R} \right)^2 \quad (191)$$

This inequality is used in [29]. To prove this write  $y = \sum_R P_R C_R$ . Then

$$\begin{aligned} y &= \sum_S P_S \sum_R P_R C_R \\ &= \sum_R \sum_S P_S P_R C_R \\ &= \sum_R P_R^2 C_R + \sum_R \sum_S (1 - \delta_{RS}) P_S P_R C_R \end{aligned} \quad (192)$$

Also, write  $z = \left( \sum_R P_R \sqrt{C_R} \right)^2$ . Then

$$\begin{aligned}
z &= \left( \sum_S P_S \sqrt{C_S} \right) \left( \sum_R P_R \sqrt{C_R} \right) \\
&= \sum_R \sum_S P_S P_R \sqrt{C_S} \sqrt{C_R} \\
&= \sum_R P_R^2 C_R + \sum_R \sum_S (1 - \delta_{RS}) P_S P_R \sqrt{C_S} \sqrt{C_R}
\end{aligned} \tag{193}$$

so that

$$\begin{aligned}
y - z &= \sum_R \sum_S P_S P_R (1 - \delta_{RS}) \left( C_R - \sqrt{C_S} \sqrt{C_R} \right) \\
&= \frac{1}{2} \sum_R \sum_S P_S P_R (1 - \delta_{RS}) \left( C_R + C_S - 2\sqrt{C_S} \sqrt{C_R} \right) \\
&= \frac{1}{2} \sum_R \sum_S P_S P_R (1 - \delta_{RS}) \left( \sqrt{C_R} - \sqrt{C_S} \right)^2 \\
&\geq 0
\end{aligned} \tag{194}$$

which proves the result.

## 10 Appendix 2 - Particle and Mode Entanglement

It is useful to contrast the two meanings of entanglement - mode and particle - in terms of three examples. The first is from the textbook by Peres ([5], see pp126-128). A system with  $N = 2$  identical particles has one particle in a single particle state (mode)  $|u\rangle$ , the other in an orthogonal single particle state  $|v\rangle$ . In first quantization the symmetrized quantum pure states for identical bosons or for identical fermions are (my notation) are

$$\begin{aligned} |\Psi\rangle_{boson} &= \frac{1}{\sqrt{2}}(|u(1)\rangle \otimes |v(2)\rangle + |u(2)\rangle \otimes |v(1)\rangle) \\ |\Psi\rangle_{fermion} &= \frac{1}{\sqrt{2}}(|u(1)\rangle \otimes |v(2)\rangle - |u(2)\rangle \otimes |v(1)\rangle) \end{aligned} \quad (195)$$

which consequently means that "two particles of the same type are always entangled". Peres obviously considers such entanglement is a result of *symmetrization*. In second quantization the state in both the fermion and boson cases is  $|1\rangle_u \otimes |1\rangle_v$  which is a separable state for modes  $u, v$ , and not a (mode) entangled state.

The second example is taken from the paper of Hyllus et al [44], specifically a case illustrated in Fig 1(b) which shows a state with  $N = 5$  identical bosons. The bosons may occupy differing spatial states (eg harmonic oscillator states) - referred to by Hyllus et al as *external* degrees of freedom - and each bosonic particle has two distinct internal states (eg hyperfine states) - *internal* degrees of freedom. Fig 1(b) shows two spatial states and two internal states ( $u, d$  say), with only the lower spatial state ( $\phi_0$  say) being occupied by  $N = 5$  bosons. From the Hyllus et al viewpoint (see last para on p 012337-4) "For indistinguishable particles, only two possibilities are allowed in this case: either ALL the *particles* are in a separable state (that is, product  $|\phi\rangle^{\otimes N}$ ) state, or all *particles* are entangled due to the *symmetrization*." Hyllus et al describe the states in terms of first quantization but for purposes of comparison we will also describe them via second quantization. What they mean by the *separable* state is in full

$$|\phi\rangle^{\otimes N} = |\phi_1\rangle |\phi_2\rangle |\phi_3\rangle |\phi_4\rangle |\phi_5\rangle \quad (196)$$

where for the  $i$ th particle the single particle space-spin state would of the form

$$|\phi_i\rangle = (\cos \theta |u_i\rangle + \sin \theta \exp i\chi |d_i\rangle) \otimes |\phi_{0i}\rangle \quad (197)$$

in which a particular internal state is chosen. The separable state in Eq.(196) is just a tensor product of single particle states for the five bosons. It is symmetric, so the symmetrization principle is satisfied. There is of course one other orthogonal separable state  $|\xi\rangle^{\otimes N} = |\xi_1\rangle |\xi_2\rangle |\xi_3\rangle |\xi_4\rangle |\xi_5\rangle$  with an orthogonal single particle space-spin state  $|\xi_i\rangle = (-\sin \theta |u_i\rangle + \cos \theta \exp i\chi |d_i\rangle) \otimes |\phi_{0i}\rangle$  in which the internal state is orthogonal to the previous one. If one of the bosons is taken from a state  $|\phi\rangle$  and placed in the orthogonal state  $|\xi\rangle$ , then representing it in

the form of a single tensor product such as  $|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_5\rangle$  would not satisfy the symmetrization principle. If one such product as  $|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_5\rangle$  is subjected to an operator which is the sum of all permutation operators  $\hat{P}$ , then apart from normalising factor the result will represent the situation where one of the five bosons is in the state  $|\xi\rangle$  rather than  $|\phi\rangle$ . Hence such a state is given by

$$\begin{aligned} |\Psi_{4,1}\rangle &= \mathcal{N} \sum_P \hat{P} (|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_5\rangle) \\ &= \mathcal{N}^\# \left( \begin{aligned} &|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_5\rangle + |\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_5\rangle|\xi_4\rangle + |\phi_1\rangle|\phi_2\rangle|\phi_5\rangle|\phi_4\rangle|\xi_3\rangle \\ &+ |\phi_1\rangle|\phi_5\rangle|\phi_3\rangle|\phi_4\rangle|\xi_2\rangle + |\phi_5\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_1\rangle \end{aligned} \right) \\ &= \mathcal{N}^\# \left( \begin{aligned} &|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_5\rangle + |\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\xi_4\rangle|\phi_5\rangle + |\phi_1\rangle|\phi_2\rangle|\xi_3\rangle|\phi_4\rangle|\phi_5\rangle \\ &+ |\phi_1\rangle|\xi_2\rangle|\phi_3\rangle|\phi_4\rangle|\phi_5\rangle + |\xi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\phi_5\rangle \end{aligned} \right) \end{aligned} \quad (198)$$

which are where the sum is over the 5! permutation operators and the  $\mathcal{N}'$ s are normalising factors. However, Hyllus et al refer to this as *entanglement by symmetrization* and regard this state as being entangled. From this point of view it is symmetrization via  $\sum_P \hat{P}$  that is responsible for entanglement in that

it creates contributions to the state vector which becomes no longer just a simple product. There is a term  $|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\xi_5\rangle$  followed by  $|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\xi_4\rangle|\phi_5\rangle$  in which particles 4 and 5 are in different single particle states.

However, from the opposing point of view in which it is modes, not particles that are entangled, and the state just described would *not* be regarded as being entangled. The Fig 1(b) case would be seen as a *two mode* situation in which the two modes are  $|U\rangle = |u\rangle \otimes |\phi_0\rangle$  and  $|D\rangle = |d\rangle \otimes |\phi_0\rangle$ . In second quantization the *Fock states* are  $|n_U, n_D\rangle = |n_U\rangle \otimes |n_D\rangle$  with  $n_U, n_D$  being the mode occupancies. It is these two modes that may or may not be entangled, and there are *six* separable pure states (*not* two) with a total of  $N = 5$  bosons, namely  $|5, 0\rangle$ ,  $|4, 1\rangle$ ,  $|3, 2\rangle$ ,  $|2, 3\rangle$ ,  $|1, 4\rangle$ , and  $|0, 5\rangle$ . The states  $|5, 0\rangle$  and  $|0, 5\rangle$  are of course equivalent in first quantization to  $|\phi_1\rangle|\phi_2\rangle|\phi_3\rangle|\phi_4\rangle|\phi_5\rangle$  and  $|\xi_1\rangle|\xi_2\rangle|\xi_3\rangle|\xi_4\rangle|\xi_5\rangle$ , whilst the state in the last equation is just the *separable* state  $|4, 1\rangle$ . The general *mode entangled* pure state with  $N = 5$  bosons is given by

$$\begin{aligned} |\Psi\rangle &= \mathcal{D}_{5,0} |5, 0\rangle + \mathcal{D}_{4,1} |4, 1\rangle \\ &\quad + \mathcal{D}_{3,2} |3, 2\rangle + \mathcal{D}_{2,3} |2, 3\rangle \\ &\quad + \mathcal{D}_{1,4} |1, 4\rangle + \mathcal{D}_{0,5} |0, 5\rangle \end{aligned}$$

where the  $\mathcal{D}$  are expansion coefficients, which is of course equivalent to various first quantization expressions. But now we would say it is the two modes  $|U\rangle$  and  $|D\rangle$  that are entangled, not the 5 bosons! Entanglement for  $N = 5$  boson pure states is associated with there being *six* distinct Fock states that occur for *five* bosons being split between *two* modes. If there were four modes then for  $N = 5$  boson pure states there would be many more distinct Fock states available depending on how the bosons are divided amongst the modes. It is

more a question of *combinatorics* rather than *symmetrization* which is relevant in determining the *dimension* of the space of entangled states. A quite different picture of what is meant by an entangled state occurs when entanglement refers to modes rather than particles.

Finally, the concept of particle entanglement is introduced somewhat differently by Wiseman et al [19].

## 11 Appendix 3 - Reference Frames and Super-Selection Rules

Several papers such as [37], [39], [26], [31], [16], [32], [33] explain the link between *reference frames* and *super-selection rules* (SSR). In this Appendix we present the key ideas involved.

### 11.1 Two Observers and Reference Frames

The first point to appreciate is that there are *two observers* - Alice and Charlie - who are involved in describing the *same state* of a particular *quantum system*. Charlie is the *external* observer, Alice the *internal* observer - perhaps closely linked to the system. It is important to realise that it is *Charlie's description* of the quantum state which is of *most interest*, in particular how this description may differ from what Alice may regard as the system state. The system could be a *multi-mode* system involving identical particles, it could just be a *single mode* system or it could even be a *single particle* with or without spin. Alice and Charlie each describe quantum states in terms of their own *reference frames*, which might be a set of *coordinate axes* for the case of the spin or position states for the single particle system, or it could be a *large quantum system* with a well-defined reference *phase* in the case of multi-mode or single mode systems involving identical particles. Alice and Charlie may each choose from a set of possible reference frames - for the single particle case there are an infinite number of difference choices of coordinate axes for example, related to each other via *rotations* and/or *translations*. In *Situation A* - which *is not* associated with *SSR* - Alice and Charlie *do know* the relationship between their two reference frames (and can communicate this relationship via *classical communications*) - such as in the case of the single particle system when the relative orientation of their two different coordinate axes are known. In *Situation B* - which *is* associated with *SSR* - Alice and Charlie *do not know* the relationship between their two reference frames - such as in the multi-mode or single mode system involving identical particles when the relative phase between their two large quantum phase reference systems is not known. Alice and Charlie describe the same state via density operators  $\hat{\sigma}$  and  $\hat{\rho}$ , and the key question is the *relationship* between these two operators in situations A and B and for various types of reference frames. In terms of the notation in [26]  $\rho \rightarrow \hat{\sigma}$  and  $\tilde{\rho} \rightarrow \hat{\rho}$ .

### 11.2 Symmetry Group

A particular relationship going from Alice's to Charlie's reference frame is specified by the *parameter*  $g$ , which in turn defines a *unitary transformation operator*  $\hat{T}(g)$  that acts in the system space. Particular examples will be listed below. If there was a third observer - Donald - and the relationship going from Charlie's to Donald's reference frame is specified by the parameter  $h$ , which in turn defines a unitary operator  $\hat{T}(h)$ , then if we symbolise the relationship going from Alice's to Donald's reference frame by the parameter  $hg$ , it follows that

$\hat{T}(hg) = \hat{T}(h)\hat{T}(g)$ . This shows that the unitary operators satisfy one of the requirements to constitute a *group*, referred to generally as the *transformation* group. The other requirements are easily confirmed. The unitary operator  $\hat{T}(0) = \hat{1}$  corresponding to the case where no change of reference frame occurs (specified by the parameter 0) exists, and satisfies the requirement that  $\hat{T}(0g) = \hat{T}(0)\hat{T}(g) = \hat{T}(g0) = \hat{T}(g)\hat{T}(0)$ . The unitary operator  $\hat{T}(g^{-1}) = \hat{T}(g)^\dagger$  corresponding to the relationship specified as  $g^{-1}$  that converts Charlie's reference frame back to that of Alice exists, and satisfies the requirement that  $\hat{T}(0) = \hat{T}(g^{-1})\hat{T}(g) = \hat{T}(g)\hat{T}(g^{-1})$ . Hence all the group properties are satisfied.

A few examples are as follows:

1. *Translation group* - single spinless particle system, with  $\hat{p}$ ,  $\hat{x}$  the momentum, position vector operators. Here  $\underline{a}$  is a vector giving the translation of Charlie's cartesian axes reference frame from that of Alice, thus  $g \equiv \underline{a}$ . The unitary translation operator is  $\hat{T}(\underline{a}) = \exp(i\hat{p} \cdot \underline{a}/\hbar)$ .

2. *Rotation group* - single particle system, with  $\hat{J}$  the angular momentum vector operators. Here  $\underline{u}$  is a unit vector giving the axis and rotation angle  $\phi$  for rotating Alice's cartesian axes reference frame into that of Charlie, thus  $g \equiv \underline{u}, \phi$ . The unitary rotation operator is  $\hat{T}(\underline{u}, \phi) = \exp(i\phi\hat{J} \cdot \underline{u}/\hbar)$ .

3. *Particle number  $U(1)$  group* - single mode bosonic system, with  $\hat{a}$  the mode annihilation operator and  $\hat{N}_a = \hat{a}^\dagger\hat{a}$  the mode number operator. Here  $\theta_a$  is the phase change Alice's to Charlie's reference frame. The unitary operator is  $\hat{T}(\theta_a) = \exp(i\hat{N}_a\theta_a)$ .

4. *Particle number  $U(1)$  group* - multi-mode bosonic system, with  $\hat{a}$  as a typical mode annihilation operator and  $\hat{N} = \sum_a \hat{a}^\dagger\hat{a}$  the total number operator.

Here  $\theta$  is the phase change from Alice's to Charlie's reference frame. The unitary operator is  $\hat{T}(\theta) = \exp(i\hat{N}\theta)$ .

In these examples the system operators  $\hat{p}$ ,  $\hat{J}$ ,  $\hat{N}_a$ ,  $\hat{N}$  etc are the *generators* of the respective groups. In many situations the generators commute with the Hamiltonian for the system (or more generally with the evolution operator that describes time evolution of the quantum state), in which case the group of unitary operators  $\hat{T}(g)$  is the *symmetry group*, and the generators are *conserved* physical quantities.

### 11.3 Relationships - Situation A

In *Situation A*, where the relationship between the reference frames for Alice and Charlie is *known* and specified by a *single* parameter  $g$ , Alice's description of the state  $\hat{\sigma}$  is related to Charlie's description  $\hat{\rho}$  for the same state via the unitary transformation

$$\hat{\rho} = \hat{T}(g) \hat{\sigma} \hat{T}(g)^{-1} \quad (199)$$

Note that this is a *passive* transformation - no change of state is involved, just the same state being described by two different observers.



As an example, consider the *spinless particle* and the *translation* group. If  $|\underline{x}\rangle$  is a position eigenstate then  $\hat{T}(\underline{a})|\underline{x}\rangle = |\underline{x} - \underline{a}\rangle$ . A pure quantum position eigenstate described by Alice as  $\hat{\sigma} = |\Phi\rangle\langle\Phi|$  with state vector  $|\Phi\rangle = |\underline{x}\rangle$  would be described by Charlie as  $\hat{\rho} = |\Psi\rangle\langle\Psi|$  but now with  $|\Psi\rangle = |\underline{x} - \underline{a}\rangle$ , which is also a pure quantum position eigenstate but with eigenvalue  $\underline{x} - \underline{a}$ . This is as expected since Alice's cartesian axes have been translated by  $\underline{a}$  to the origin of Charlie's axes without change of orientation. In the case of momentum eigenstates  $|\underline{p}\rangle$  we have  $\hat{T}(\underline{a})|\underline{p}\rangle = \exp(i\underline{p} \cdot \underline{a}/\hbar)|\underline{p}\rangle$ , so a pure quantum momentum eigenstate described by Alice with  $|\Phi\rangle = |\underline{p}\rangle$  would be described by Charlie with  $|\Psi\rangle = \exp(i\underline{p} \cdot \underline{a}/\hbar)|\underline{p}\rangle$ , which is also a pure momentum eigenstate with the same eigenvalue  $\underline{p}$ . Alice and Charlie describe the pure momentum eigenstate with the same density operator  $\hat{\rho} = \hat{\sigma}$ , the phase factor cancels.

For more general pure states, consider a quantum state described by Alice as  $\hat{\sigma} = |\Phi\rangle\langle\Phi|$  with state vector  $|\Phi\rangle = \int d\underline{x} \phi(\underline{x}) |\underline{x}\rangle$ . States of this form can represent *localised* states when  $\phi(\underline{x})$  is only significant in confined spatial regions, or they can represent *delocalised* states such as momentum eigenstates  $|\underline{p}\rangle$  when  $\phi(\underline{x}) = (2\pi\hbar)^{-3/2} \exp(i\underline{p} \cdot \underline{x}/\hbar)$ . We see that Charlie also describes a pure quantum state  $\hat{\rho} = |\Psi\rangle\langle\Psi|$  but now with  $|\Psi\rangle = \hat{T}(\underline{a})|\Phi\rangle = \int d\underline{x} \phi(\underline{x} + \underline{a}) |\underline{x}\rangle = \int d\underline{x} \psi(\underline{x}) |\underline{x}\rangle$ , so the wavefunction is now  $\psi(\underline{x}) = \phi(\underline{x} + \underline{a})$ .

Note that if Alice's state vector was written in terms of momentum eigenstates  $|\Phi\rangle = \int d\underline{p} \tilde{\phi}(\underline{p}) |\underline{p}\rangle$ , then Charlie's state vector  $|\Psi\rangle = \int d\underline{p} \tilde{\psi}(\underline{p}) |\underline{p}\rangle$  has a momentum wave function  $\tilde{\psi}(\underline{p}) = \exp(i\underline{p} \cdot \underline{a}/\hbar) \tilde{\phi}(\underline{p})$  related to that of Alice by a phase factor. Note that a state which is a quantum superposition of momentum eigenstates as described by Alice is also described as a quantum superposition of momentum eigenstates by Charlie. A similar feature applies in all situation A cases, and is related to SSR *not* applying in situation A.

The case of the *particle* with *spin* and the *rotation* group is outlined in Ref. [39].

## 11.4 Relationships - Situation B

In *Situation B*, where on the other hand the relationship between frames is completely *unknown*, all possible transformations  $g$  must be given *equal weight*, and hence the relationship between Alice's and Charlie's description of the same

state becomes

$$\begin{aligned}\hat{\rho} &= \int w(g) dg \hat{T}(g) \hat{\sigma} \hat{T}(g)^{-1} \\ &= \mathcal{G}[\hat{\sigma}]\end{aligned}\tag{200}$$

where  $\int w(g) dg$  is a symbolic integral over the parameter  $g$ , which includes a weight factor  $w(g)$  so that  $\int w(g) dg = 1$ . This linear process connecting  $\hat{\sigma}$  to  $\hat{\rho}$  is the " $\mathcal{G}$ -twirling" operation. Again, this is a paassive transformation.

It is straightforward to show that for any fixed parameter  $h$  that

$$\hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \hat{\rho}\tag{201}$$

showing that Charlie's density operator is  $\mathcal{G}$  invariant under the transformation group - unlike the case for Situation A.

As an example, consider the *single mode* bosonic system and the  $U(1)$  group. If  $|n_a\rangle$  is a Fock state then  $\hat{T}(\theta_a) |n_a\rangle = \exp(in_a\theta_a) |n_a\rangle$ . Consider a pure quantum state described by Alice as the *Glauber coherent state*  $\hat{\sigma} = |\Phi\rangle\langle\Phi|$  with state vector  $|\Phi(\beta)\rangle = \sum_{n_a} C(n_a, \beta) |n_a\rangle$ , where  $C(n_a, \beta) = \exp(-|\beta|^2/2) \beta^{n_a} / \sqrt{(n_a)!}$ .

It is straightforward to show that

$$\hat{T}(\theta_a) |\Phi(\beta)\rangle = |\Phi(\beta \exp(i\theta_a))\rangle\tag{202}$$

so that the Glauber coherent state is transformed into another Glauber coherent state, but with  $\beta$  changed via a phase factor to  $\beta \exp(i\theta_a)$ . The quantum state described by Charlie is given by

$$\begin{aligned}\hat{\rho} &= \int \frac{d\theta_a}{2\pi} |\Phi(\beta \exp(i\theta_a))\rangle \langle\Phi(\beta \exp(i\theta_a))| \\ &= \int \frac{d\theta_a}{2\pi} \sum_{n_a} \sum_{m_a} C(n_a, \beta) C(m_a, \beta)^* \hat{T}(\theta_a) |n_a\rangle \langle m_a| \hat{T}(\theta_a)^\dagger \\ &= \sum_{n_a} \sum_{m_a} C(n_a, \beta) C(m_a, \beta)^* |n_a\rangle \langle m_a| \int \frac{d\theta_a}{2\pi} \exp(i[n_a - m_a]\theta_a) \\ &= \sum_{n_a} |C(n_a, \beta)|^2 |n_a\rangle \langle n_a| \\ &= \sum_{n_a} \exp(-|\beta|^2) \frac{(|\beta|^2)^{n_a}}{(n_a)!} |n_a\rangle \langle n_a|\end{aligned}\tag{204}$$

which is a *mixed state* consisting of a *Poisson distribution* of *Fock states* with mean occupation number  $\bar{n}_a = |\beta|^2$ . In view of the first expression for  $\hat{\rho}$  it can also be thought of as a mixed state consisting of Glauber coherent states each with the same amplitude  $|\beta| = \sqrt{\bar{n}_a}$ , but with all phases ( $\arg \beta + \theta_a$ ) equally probable. Thus, whereas Alice describes the state as a pure state that

is a quantum superposition of Fock states with differing occupancy numbers, Charlie describes the same state as a mixed state involving a statistical mixture of number states. The former violates the SSR whereas the latter does not. A similar feature applies in all situation B cases, and is related to SSR applying in Situation B. Whether Alice could ever prepare such a state in the first place is controversial - see the discussion presented above in SubSections 2.7 and 2.9. However, *assuming* she could, the quantum state as described by Charlie is a mixed state.

The situation just studied relates of course to the debate [59] regarding whether the quantum state for a *single mode laser* operating well above threshold should be described by a Glauber coherent state or as a Poisson statistical mixture of photon number states. The first viewpoint (Alice) describes the state from the point of view of an internal observer with a reference frame, the second (Charlie) describes the same state from the point of view of an external observer for whose reference frame relationship to that of the internal observer is unknown. The debate is regarded by [39] as settled on the basis that both viewpoints are valid, they are just at cross purposes because they refer to descriptions of the same quantum state by two different observers.

It should not be thought however that the quantum state would always be described in such a fundamentally different manner for all Situation B cases. As an example, consider the *multi-mode bosonic* system and the  $U(1)$  group. Consider the pure quantum state described by Alice as the multi-mode  $N$  boson *Fock state*  $\hat{\sigma} = |\Phi\rangle\langle\Phi|$  with state vector  $|\Phi(N)\rangle = |n_1 n_2 \dots n_a \dots; N\rangle = \prod_a |n_1\rangle |n_2\rangle \dots |n_a\rangle \dots$ , where  $N = \sum_a n_a$ . We have  $\hat{T}(\theta) |n_1 n_2 \dots n_a \dots; N\rangle = \exp(iN\theta) |n_1 n_2 \dots n_a \dots; N\rangle$ ,

so that the same state would be described by Charlie as  $\hat{\rho} = |\Psi\rangle\langle\Psi|$  and with  $|\Psi\rangle = |n_1 n_2 \dots n_a \dots; N\rangle$ . This is also a multi-mode  $N$  boson Fock state with exactly the same occupancies. The product  $\exp(iN\theta) \exp(-iN\theta)$  of phase factors averages out to unity and here  $\hat{\rho} = \hat{\sigma}$ , so Alice and Charlie both describe the multi-mode Fock states in the same way. Another example for *two mode bosonic* systems and the  $U(1)$  group is provided by the one boson *Bell states* (the BS notation used here is non-conventional). These are entangled two mode states that Alice would describe via the state vectors  $|\Phi^\pm\rangle = (|10\rangle \pm |01\rangle)/\sqrt{2}$ . We have  $\hat{T}(\theta) |\Phi^\pm\rangle = \exp(i\theta) |\Phi^\pm\rangle$ , so that the same state would be described by Charlie with  $|\Psi^\pm\rangle = (|10\rangle \pm |01\rangle)/\sqrt{2}$ . Again the product of phase factors averages to unity and  $\hat{\rho} = \hat{\sigma}$ , so Alice and Charlie both describe the quantum states as Bell states, and in the same form.

## 11.5 Dynamical and Measurement Considerations

Discussions of the relationship between equations governing the dynamical behaviour of Alice's and Charlie's density operators depend on whether the evolution is just governed by a Hamiltonian or whether master equations describing evolution affected by interactions with an external environment are involved. Such matters will not be treated in detail here, nor will the issue of relating

Alice's and Charlie's measurements. The latter issue is dealt with in [26].

However, in the case where Alice describes the *Hamiltonian evolution* of her density operator via the Liouville - von-Neumann equation

$$i\hbar \frac{\partial}{\partial t} \hat{\sigma} = [\hat{H}, \hat{\sigma}] \quad (205)$$

where in Alice's frame the Hamiltonian is  $\hat{H}$ , and where in addition the transformation group is also the *symmetry group* so that  $\hat{T}(g)\hat{H}\hat{T}(g)^{-1} = \hat{H}$  for all  $g$ , it is easy to see that for both Situations A and B, Charlie's density operator will evolve via the same LVN equation

$$i\hbar \frac{\partial}{\partial t} \hat{\rho} = [\hat{H}, \hat{\rho}] \quad (206)$$

Thus both Alice and Charlie will describe the same dynamical evolution, though of course the initial (and hence evolved) states may differ in the two cases.

## 11.6 Nature of Reference Frames

Reference frames of differing types are involved for the various transformation groups. The common feature is that they are thought of as *actual physical systems* themselves which are either macroscopic *classical* systems or macroscopic *quantum* systems in states associated with the *classical limit*. They are intended to be *essentially unaffected* by the presence of the systems for which they are acting as reference frames. In some cases relatively uncontroversial examples exist, such as for the *cartesian axes* associated with the *translation* and *rotation* groups associated with the single particle system. The physical reference system may be a large *magnet* whose magnetic field points in a well defined direction and defines a  $z$  axis, combined with an *electrostatic generator* whose electric field is in another well defined direction at right angles that defines an  $x$  axis. In other cases the existence of suitable reference frames is less clear.

In this SubSection we will describe possible phase reference frames as if they are entirely separated (or uncorrelated) with the system of interest. In terms of the treatment by Bartlett et al [39], [26] these are *non-implicated* reference frames. In the next SubSection and in the next Appendix phase reference frames that are correlated with the system of interest will be described - these are the so-called *implicated* reference frames of Bartlett et al.

For the large quantum system with a well-defined reference *phase* associated with the  $U(1)$  group in the case of multi-mode or single mode systems involving identical particles, the usual choice is a single mode bosonic system such as a single mode *BEC* or a *laser* with a large mean occupancy, and which is thought of as being prepared in a Glauber coherent state  $|\Phi(\alpha)\rangle$  in order to provide the *phase reference frame*, the reference phase being  $\arg \alpha$ . Whether such a reference frame really exists is controversial. The discussion presented above in SubSections 2.7 and 2.9 raises the question of whether such a phase reference state could ever be prepared, so this choice of a physical phase reference is rather

unsatisfactory. However, from the point of view of this presentation we *assume* it does, so that - as in the previous example - Alice can describe the reference state as another coherent state. Again, whether Alice could ever prepare such a state is questionable.

Another possibility for a physical phase reference is a *macroscopic* low frequency *harmonic oscillator*, whose quantum energy eigenstates  $|n\rangle$  - with  $n = 0, 1, \dots, n_{\max}$  and energies  $n\hbar\omega$  can be used to construct phase eigenstates  $|\theta_p\rangle$  with  $p = 0, 1, \dots, n_{\max}$  and  $\theta_p = p \times 2\pi/(n_{\max} + 1)$ , and which are defined by [70]

$$|\theta_p\rangle = \frac{1}{\sqrt{n_{\max} + 1}} \sum_{n=0}^{n_{\max}} \exp(in\theta_p) |n\rangle \quad (207)$$

These states are orthonormal. The separation between the equally spaced phase angles  $\Delta\theta = 2\pi/(n_{\max} + 1)$  can be made very small if  $n_{\max}$  is large enough. Under the effect of the harmonic oscillator Hamiltonian  $\hat{H} = \hbar\omega\hat{N}$ , where  $\hat{N}$  is the number operator, the phase state  $|\theta_p\rangle$  evolves into  $|\theta_p - \omega\Delta t\rangle$  during a time interval  $\Delta t$ , so if the time intervals are chosen so that  $\omega\Delta t = 2\pi/(n_{\max} + 1)$ , the phase angle  $\theta_p$  changes into  $\theta_{p-1}$ . Thus the system behaves like a backwards running *clock* [79], the phase angles  $\theta_p$  defining the positions of the hands. If the clock initially has phase  $\theta_p$  the probability of finding the clock to have phase  $\theta_q$  after a time interval  $\Delta t$  is given by

$$P(\theta_q, \theta_p, \Delta t) = \frac{1}{(n_{\max} + 1)^2} \frac{\sin^2((n_{\max} + 1)\Delta/2)}{\sin^2(\Delta/2)} \quad (208)$$

where  $\Delta = \theta_p - \theta_q - \omega\Delta t$ . For times  $\Delta t$  such that  $\omega\Delta t \ll 2\pi/(n_{\max} + 1)$  the probability of the phase remaining as  $\theta_p$  is close to unity. Thus if the phase state  $|\theta_p\rangle$  is used as a phase reference, it will remain stable for a time  $\Delta t$  satisfying the last inequality. For  $\Delta t \sim 100\mu\text{s}$  and  $n_{\max} \sim 10^4$  so that phase is defined to  $\sim 10^{-3}$  radians, an oscillator frequency  $\omega \sim 10^0 \text{ s}^{-1}$  would suffice for this phase reference standard. Such macroscopic oscillators do exist, though the process to prepare them in the phase reference *quantum* state  $|\theta_p\rangle$  would be technically difficult. Whether such a system would be useful as a phase reference for optical fields or a BEC is another issue

## 11.7 Relational Description of Phase References

In this SubSection phase reference frames that are correlated with the system of interest will be described - these are the so-called *implicated* reference frames of Bartlett et al [39], [26].

One such approach to describing phase references in the  $U(1)$  group case is via the concept of *maps*. For simplicity consider a one mode system  $S$ , the basis vectors for which are Fock states  $|m\rangle_S$ , where it is sufficient to restrict  $m = 0, 1, \dots, m_{\max}$ . The reference system  $R$ , will also be a one mode system with Fock states  $|n\rangle_R$ , where  $n$  is large. Product states  $|m\rangle_S \otimes |n\rangle_R$  for the combined modes exist in the Hilbert space  $H_S \otimes H_R$  and are eigenstates of the

various number operators, including the total number operator  $\hat{N}_T = \hat{N}_S + \hat{N}_R$  - where the eigenvalue is  $l = m + n$ . The product states may be listed via  $m = 0, 1, \dots, m_{\max}$  and  $n = 0, 1, \dots$  or  $m = 0, 1, \dots, m_{\max}$  and  $l = m, m + 1, \dots$ . Here we will describe how a *coherent superposition of number states*, such as a Glauber coherent state can be represented.

In the so-called *internalisation* or *quantisation* of the reference frame the product state  $|m\rangle_S \otimes |n\rangle_R$  is mapped onto the product state  $|m\rangle_S \otimes |n - m\rangle_R$  where  $n \geq m_{\max}$ . Thus

$$|m\rangle_S \otimes |n\rangle_R \rightarrow |m\rangle_S \otimes |n - m\rangle_R \quad (209)$$

Hence for a linear combination of system states given by

$$|\Phi\rangle_S = \sum_{m=0}^{m_{\max}} C_m |m\rangle_S \quad (210)$$

we have for the state  $|\Phi\rangle_S \otimes |n\rangle_R$  in  $H_S \otimes H_R$

$$|\Phi\rangle_S \otimes |n\rangle_R = \sum_{m=0}^{m_{\max}} C_m |m\rangle_S \otimes |n\rangle_R \rightarrow \sum_{m=0}^{m_{\max}} C_m |m\rangle_S \otimes |n - m\rangle_R = |\Psi_n\rangle_{RS} \quad (211)$$

The mapping results in an entangled state where there are  $n$  bosons distributed between the two modes. This state  $|\Psi_n\rangle_{RS}$  is a pure state which is compatible with the SSR and is in one-one correspondence with the original system state  $|\Phi\rangle_S$ . Note that to create this state the reference state  $|n\rangle_R$  must have more bosons in it than  $m_{\max}$ . The density operator for the original pure system  $S$  state would be  $\hat{\sigma}_S = |\Phi\rangle_S \langle \Phi|_S$ , and we note that this state violates the SSR. The state  $|\Phi\rangle_S$  would be essentially a Glauber coherent state if  $C_m = \exp(-|\alpha|^2/2) \alpha^m / (\sqrt{m!})$ , with  $m_{\max} \gg |\alpha|^2$ . However, for the mapped state  $|\Psi_n\rangle_{RS}$  the reduced density operator  $\hat{\rho}_S$  is given by

$$\begin{aligned} \hat{\rho}_S &= \text{Tr}_R(|\Psi_n\rangle_{RS} \langle \Psi|_{RS}) \\ &= \sum_{m=0}^{m_{\max}} |C_m|^2 |m\rangle_S \langle m|_S \end{aligned} \quad (212)$$

This is a mixed state and is compatible with the SSR. For the Glauber coherent state  $|\Phi\rangle_S$  this is the Poisson distribution of number states. Hence the original SSR violating superposition of number states for system  $S$  is mapped onto a state in the combined system for which the reduced density operator is a statistical mixture and is consistent with the SSR.  $\hat{\sigma}_S$  would correspond to Alice's description of the state,  $\hat{\rho}_S$  to Charlie's.

In the alternative so-called *externalisation* of the reference frame the mapping is between product states, and is the reverse of the previous mapping. The product state  $|m\rangle_S \otimes |n\rangle_R$  is mapped onto the product state  $|m\rangle_S \otimes |m + n\rangle_R$  in the Hilbert space  $H_S \otimes H_R$  where the former is spanned by vectors  $|m\rangle_S$  and the latter by vectors  $|m + n\rangle_R$ , and where  $n \geq m_{\max}$ . Thus

$$|m\rangle_S \otimes |n\rangle_R \rightarrow |m\rangle_S \otimes |m + n\rangle_R \quad (213)$$

The mapping of the  $H_S \otimes H_R$  state  $|\Psi_n\rangle_{RS}$  then is

$$\begin{aligned} |\Psi_n\rangle_{RS} &= \sum_{m=0}^{m_{\max}} C_m |m\rangle_S \otimes |n-m\rangle_R \\ &\rightarrow \sum_{m=0}^{m_{\max}} C_m |m\rangle_S \otimes |n\rangle_R = \left( \sum_{m=0}^{m_{\max}} C_m |m\rangle_S \right) \otimes |n\rangle_R = |\Xi_n\rangle_{RS} \end{aligned} \quad (214)$$

The mapping results in a non-entangled state which is incompatible with the SSR. The state in the subspace  $H_S$  is a coherent superposition of number states, whilst that in  $H_R$  is a Fock state. The reduced density operator in  $H_S$  is  $\hat{\sigma}_S^\#$  given by

$$\begin{aligned} \hat{\sigma}_S^\# &= \text{Tr}_R(|\Xi_n\rangle_{RS} \langle \Xi_n|_{RS}) \\ &= \sum_{m=0}^{m_{\max}} \sum_{k=0}^{m_{\max}} C_m C_k^* |m\rangle_S \langle k|_S \end{aligned} \quad (215)$$

which is the same as  $\hat{\sigma}_S = |\Phi\rangle_S \langle \Phi|_S$  and involves coherences between different number states in contradiction to the SSR. Clearly this second mapping just reverses the first one.

Of these two treatments of phase reference frames, the internalisation version has a closer link to physics in that the pure state  $|\Psi_n\rangle_{RS}$  can in principle be created and does lead to a way of creating a state that is in one-one correspondence with any SSR violating pure state  $|\Phi\rangle_S$ , though it is in the form of an entangled state of the  $S$ ,  $R$  sub-systems rather than just  $S$  alone. This is an important point to note - the original SSR violating state does not exist as a state of a separate system, all that exists is an SSR compatible entangled state that is in one-one correspondence with it. However, the general process for creating a state such as  $|\Psi_n\rangle_{RS}$  is not explained. For simple cases such as  $|\Phi\rangle_S = (|0\rangle_S + |1\rangle_S)/\sqrt{2}$  the creation of the required state  $|\Psi_n\rangle_{RS} = (|0\rangle_S \otimes |n\rangle_R + |1\rangle_S \otimes |n-1\rangle_R)/\sqrt{2}$ , where  $n \geq 1$  would seem feasible via the ejection of one boson from a BEC in a Fock state  $|n\rangle_R$  into a previously unoccupied mode. .

## 11.8 Irreducible Matrix Representations and Super-selection Rules

If  $|i\rangle$  ( $i = 1, 2, \dots$ ) are a set of orthonormal basis vectors in the system state space, then the group of unitary operators  $\hat{T}(g)$  is represented by a group of *unitary matrices*  $D(g)$

$$\hat{T}(g) |i\rangle = \sum_j D_{ji}(g) |j\rangle \quad (216)$$

with elements  $D_{ji}(g)$ , and such that  $D(hg) = D(h)D(g)$  etc corresponding to the group properties of the operators. This is a *matrix representation* of the transformation group.

The theory of such group representations and their application to quantum systems is well established, following the pioneering work of Wigner in the 1930s. We can just use the results here. A key concept is that of *irreducible* representations. Within the system state space we can in general choose so-called irreducible sub-spaces, denoted as  $\Gamma_\alpha$  of dimension  $d_\alpha$  and spanned by new orthonormal basis vectors  $|\Gamma_\alpha\lambda\rangle$  ( $\lambda = 1, 2, \dots, d_\alpha$ ) such that

$$\hat{T}(g) |\Gamma_\alpha\lambda\rangle = \sum_{\mu=1}^{d_\alpha} D_{\mu\lambda}^\alpha(g) |\Gamma_\alpha\mu\rangle \quad (217)$$

For each irreducible sub-space  $\Gamma_\alpha$  there is *no* smaller sub-space for which the operation of all  $\hat{T}(g)$  just leads to linear combinations of vectors within that sub-space. The  $d_\alpha \times d_\alpha$  matrices  $D^\alpha(g)$  then form an irreducible matrix representation for the transformation group. For different  $\alpha$  the representations are said to be *inequivalent*.

The irreducible matrices satisfy the so-called *great orthogonality theorem* [80]

$$\int w(g) dg D_{\mu\lambda}^\alpha(g) D_{\xi\tau}^\beta(g)^* = \frac{1}{d_\alpha} \delta_{\alpha\beta} \delta_{\mu\xi} \delta_{\lambda\tau} \quad (218)$$

The proof of this result is based on Schur's lemma.

The importance of the irreducible representations and the consequent orthogonality theorem lies in its application to Situation B cases, where we have seen that Charlie's density operator  $\hat{\rho}$  is invariant under any of the transformations  $\hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} = \hat{\rho}$ . Suppose we represent  $\hat{\rho}$  in terms of the basis vectors  $|\Gamma_\alpha\lambda\rangle$  associated with the irreducible representations

$$\hat{\rho} = \sum_{\alpha\lambda} \sum_{\beta\tau} R_{\lambda\tau}^{\alpha\beta} |\Gamma_\alpha\lambda\rangle \langle\Gamma_\beta\tau| \quad (219)$$

where  $R$  will be a Hermitian, positive definite matrix with unit trace since it represents a density operator. Applying the transformation gives

$$\begin{aligned} \hat{T}(h) \hat{\rho} \hat{T}(h)^{-1} &= \sum_{\alpha\lambda\mu} \sum_{\beta\tau\xi} R_{\lambda\tau}^{\alpha\beta} D_{\mu\lambda}^\alpha(h) |\Gamma_\alpha\mu\rangle \langle\Gamma_\beta\tau| D_{\xi\tau}^\beta(h)^* \\ &= \hat{\rho} \end{aligned} \quad (220)$$

Averaging over  $h$  and using the great orthogonality theorem gives

$$\hat{\rho} = \sum_{\alpha} \sum_{\mu} \left( \sum_{\lambda} \frac{1}{d_\alpha} R_{\lambda\lambda}^{\alpha\alpha} \right) |\Gamma_\alpha\mu\rangle \langle\Gamma_\alpha\mu| \quad (221)$$

This is in the form of a mixed state involving irreducible state vectors  $|\Gamma_\alpha\mu\rangle$  each occuring with a probability  $P_\mu^\alpha$  given by

$$P_\mu^\alpha = \sum_{\lambda} \frac{1}{d_\alpha} R_{\lambda\lambda}^{\alpha\alpha} = P^\alpha \quad (222)$$



which is the same for all  $\mu$  associated with a given irreducible representation  $\Gamma_\alpha$ . This is clearly a positive real quantity and since

$$\begin{aligned} \sum_\alpha \sum_\mu P_\mu^\alpha &= \sum_\alpha \sum_\mu \sum_\lambda \frac{1}{d_\alpha} R_{\lambda\lambda}^{\alpha\alpha} = \sum_\alpha \sum_\lambda R_{\lambda\lambda}^{\alpha\alpha} \\ &= \text{Tr } \hat{\rho} = 1 \end{aligned} \quad (223)$$

the probabilities sum to unity as required.

The final result for Charlie's density operator

$$\hat{\rho} = \sum_\alpha \sum_\mu P^\alpha |\Gamma_\alpha \mu\rangle \langle \Gamma_\alpha \mu| \quad (224)$$

demonstrates the presence of a *super-selection rule*. In Charlie's description of the quantum state there are *no coherences* between states  $|\Gamma_\alpha \mu\rangle$  associated with differing irreducible representations of the transformation group. This represents the general form of the SSR for all transformation groups in Situation B cases.

As an example, consider the  $U(1)$  group and the *single mode* bosonic system. Since the Fock states satisfy  $\hat{T}(\theta_a) |n_a\rangle = \exp(in_a \theta_a) |n_a\rangle$  they form the basis for the irreducible representations of the  $U(1)$  group, the occupation number  $n_a$  specifying the irreducible representation and the  $1 \times 1$  matrices  $\exp(in_a \theta_a)$  being the unitary matrices. Hence Charlie will describe the quantum state as

$$\hat{\rho} = \sum_{n_a} P(n_a) |n_a\rangle \langle n_a| \quad (225)$$

which is a statistical mixture of Fock states with no coherences between different Fock states. This result is of the same form as in Eq.(46) and is in accord with the SSR on boson number.

As another example, consider the  $U(1)$  group and the *multi-mode* bosonic system. Here sums of products of Fock states

$$|n_1 n_2 \dots n_a \dots; N\rangle = \prod_a |n_1\rangle |n_2\rangle \dots |n_a\rangle \dots \quad N = \sum_a n_a \quad (226)$$

such that the total occupancy is  $N = \sum_a n_a$  can be used to form irreducible representations for the transformation group in terms of linear combinations of the products with the same  $N$ . Writing these linear combinations as

$$|\Psi_N^\mu\rangle = \sum_{\{n_1 n_2 \dots n_a \dots\}} C_{\{n_1 n_2 \dots n_a \dots\}}^{N\mu} |n_1 n_2 \dots n_a \dots; N\rangle \quad (227)$$

we have since  $\hat{T}(\theta) |n_1 n_2 \dots n_a \dots; N\rangle = \exp(iN\theta) |n_1 n_2 \dots n_a \dots; N\rangle$  we see that  $\hat{T}(\theta) |\Psi_N^\mu\rangle = \exp(iN\theta) |\Psi_N^\mu\rangle$  also, so the  $|\Psi_N^\mu\rangle$  define the irreducible basis states. The total occupancy  $N$  specifies the irreducible representation, but here there

are many irreducible representations with the same  $N$  depending on the various  $\mu$ . In this case Charlie will describe the state as

$$\hat{\rho} = \sum_N \sum_{\mu} P_{\mu}^N |\Psi_N^{\mu}\rangle \langle \Psi_N^{\mu}| \quad (228)$$

which is a statistical mixture of multi-mode states  $|\Psi_N^{\mu}\rangle$  all with the same total occupancy  $N$ . Although there are coherence terms between individual modal Fock states, there are no coherences between states with different total occupancy. This result is of the same form as in Eq.(27) and again is an example of a super-selection rule operating in terms of Charlie's description of the quantum state.

Finally, we note that in situation A where the relationship between the frames is known and there is no invariance for Charlie's density operator, we do not have SSR applying. For the *single particle* case and the *translation group* the momentum states  $|\underline{p}\rangle$  define the irreducible representations, each specified by  $\underline{p}$ , and as we saw Charlie's description of the quantum state involved linear combinations of these irreducible basis vectors, in contradiction to the SSR.

## 11.9 Non-Entangled States

The essential feature of an *non-entangled* or *separable* state is that the sub-systems are considered to be *unrelated* to each other. Hence, both for Alice and Charlie there will be *separate reference frames* for each sub-system, with transformation groups -  $\hat{T}_A(g_a)$  for sub-system  $A$ ,  $\hat{T}_B(g_b)$  for sub-system  $B$ , etc which relate the reference systems of Alice to those of Charlie. The transformations  $g_a, g_b, ..$  are different. The *overall* transformation operator would be of the form  $\hat{T}(g_a, g_b, ..) = \hat{T}_A(g_a) \otimes \hat{T}_B(g_b) \otimes ...$  Alice would describe a general non-entangled state as having a density operator

$$\hat{\sigma} = \sum_R P_R \hat{\sigma}_R^A \otimes \hat{\sigma}_R^B \otimes \hat{\sigma}_R^C \otimes ... \quad (229)$$

It then follows for Situation B where the reference frames for Alice and Charlie are unrelated, that Charlie would describe the same state via the density operator

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^A \otimes \hat{\rho}_R^B \otimes \hat{\rho}_R^C \otimes ... \quad (230)$$

where

$$\hat{\rho}_R^C = \int w(g_c) dg_c \hat{T}_C(g_c) \hat{\sigma}_R^C \hat{T}_C(g_c)^{-1} \quad C = A, B, .. \quad (231)$$

Note that *separate* twirl operations are applied to the different sub-systems, as explicitly shown in the papers by Vaccaro et al [31] (see Section IIIA, Eqn. 3.3 therein) and Paterek et al [33] (see Section 6). This leads for general transformation groups to the *local group super-selection rule*, where the  $\hat{\rho}_R^C$  involve

*no coherences* between states associated with differing irreducible representations of the transformation group. We see that Charlie also describes a non-entangled state and with the same mixture probability  $P_R$  as for Alice. Thus non-entanglement or separability is a feature that is the *same* for both Alice and Charlie, as ought to be the case.

In the context of sub-systems consisting of *modes* (or sets of modes) occupied by *identical bosons*, the case of interest is Situation B, with each transformation group being  $U(1)$ . Here the relationship between Charlie's and Alice's *phase reference* frames are unknown. Hence irrespective of Alice's description of the sub-system states  $\hat{\sigma}_R^A, \hat{\sigma}_R^B, \dots$  we see from the previous section that Charlie will describe the separate sub-system states  $\hat{\rho}_R^A, \hat{\rho}_R^B$ , as statistical mixtures of number states for the separate modes (or total number states for the sets of modes in each sub-system). Thus from Charlie's point of view the separate mode density operators will satisfy the SSR. Thus we see that the introduction of reference frames and two observers - Charlie being the external one whose description of the quantum states is of primary interest - leads to the *same SSR outcome* as the simpler considerations set out in SubSections 2.7 and 2.9. Essentially the same considerations have been used in [25], [31] and the other papers to justify the *local photon number superselection rule*.

## 12 Appendix 4 - Super-Selection Rule Violations ?

### 12.1 Preparation of Coherent Superposition of an Atom and a Molecule ?

A key paper dealing with the coherent superposition of an atom and a molecule is that by Dowling et al [62], entitled “Observing a coherent superposition of an atom and a molecule”. Essentially the process involves one atom A interacting with a BEC of different atoms B leading to the creation of one molecule AB, with the BEC being depleted by one B atom.

#### 12.1.1 Hamiltonian

The Hamiltonian is given by

$$\hat{H} = \hbar\omega_A \hat{b}_A^\dagger \hat{b}_A + \hbar\omega_M \hat{b}_M^\dagger \hat{b}_M + \hbar\omega_2 \hat{b}_2^\dagger \hat{b}_2 + \frac{\hbar\kappa}{2} (\hat{b}_M^\dagger \hat{b}_A \hat{b}_2 + \hat{b}_M \hat{b}_A^\dagger \hat{b}_2^\dagger) \quad (232)$$

where  $\hat{b}_A, \hat{b}_M$  and  $\hat{b}_2$  are standard bosonic annihilation operators for the atom, molecule and BEC modes respectively,  $\omega_A, \omega_M$  and  $\omega_2$  are the corresponding mode frequencies and  $\kappa$  defines the interaction strength for the process where a molecule is created or destroyed from/to an atom A and a BEC atom B.  $\Delta$  is the frequency difference between the molecular state AB and the two separate states for atoms A and B – this is zero on Feshbach resonance - and is given by

$$\Delta = \omega_M - \omega_A - \omega_2 \quad (233)$$

The Hamiltonian commutes with the total number operator  $\hat{N}_{tot}$ , where

$$\hat{N}_{tot} = 2\hat{b}_M^\dagger \hat{b}_M + \hat{b}_A^\dagger \hat{b}_A + \hat{b}_2^\dagger \hat{b}_2 \quad (234)$$

where the molecule number operator is multiplied by two.

#### 12.1.2 Initial State

Initially the state of the system is given by the density operator Eqs (10) and (11) in the paper

$$\widehat{W}_{0L} = \int \frac{d\theta}{2\pi} \exp(-i\hat{N}_{tot}\theta) |\Psi\rangle_{0L} \langle\Psi|_{0L} \exp(+i\hat{N}_{tot}\theta) \quad (235)$$

$$|\Psi\rangle_{0L} = |A\rangle |\beta\rangle \quad (236)$$

where  $|A\rangle$  is a state with one atom A and  $|\beta\rangle$  is a Glauber coherent state for the BEC of atoms B. The super-operator acting on the pure state  $|\Psi\rangle_{0L} \langle\Psi|_{0L}$  is called the *twirling operator*, the group of unitary operators  $\exp(-i\hat{N}_{tot}\theta)$  depend on a *phase* variable  $\theta$  and are a unitary representation of  $U(1)$ , the *generator*

being  $\hat{N}_{tot}$ . These operators act as a *symmetry group* for the system and leave the Hamiltonian invariant. The *initial state* is also given by

$$\widehat{W}_{0L} = \hat{\rho}_{A-M}(0) \otimes \hat{\rho}_2(0) \quad (237)$$

$$\hat{\rho}_{A-M}(0) = |A\rangle \langle A| \quad (238)$$

$$\hat{\rho}_2(0) = \int \frac{d\theta}{2\pi} \exp(-i\hat{n}_2\theta) |\beta\rangle \langle\beta| \exp(+i\hat{n}_2\theta) \quad (239)$$

$$= \sum_n p_n(< n >) |n\rangle \langle n| \quad (240)$$

$$= \int \frac{d\theta}{2\pi} |\beta \exp(-i\theta)\rangle \langle\beta \exp(-i\theta)| \quad (241)$$

where  $\hat{n}_2 = \hat{b}_2^\dagger \hat{b}_2$  is the number uperator for the BEC mode and  $p_n(< n >) = \{\exp(-< n >) < n >^n / n!\}$  is a Poisson distribution, whose mean is  $< n > = |\beta|^2$ . Initially then there is one atom A and the BEC is in a statistical mixture of number states with a Poisson distribution, which is mathematically equivalent to a statistical mixture of Glauber coherent states  $|\beta \exp(-i\theta)\rangle$  with the same amplitude  $\sqrt{< n >}$  but with all phases ( $\arg \beta + \theta$ ) being equally weighted.

### 12.1.3 Implicated Reference Frame

In the paper by Dowling et al [62] the BEC is acting as an *implicated phase reference frame* (see [39], [26]). The state of the reference frame as described by Charlie is given by

$$\hat{\rho}_{REF} = \hat{\rho}_2(0) = \int \frac{d\theta}{2\pi} \exp(-i\hat{n}_2\theta) |\beta\rangle \langle\beta| \exp(+i\hat{n}_2\theta) \quad (242)$$

and from Eq. (232), there is an interaction between the reference BEC and the separate atom A and molecule M systems. However, because  $< n > = |\beta|^2$  is very large, the BEC is essentially unchanged during the process, as reflected in the use of approximations in eqs (27), (28) of the paper. Another implicated phase reference frame situation, but involving a two mode reference frame is discussed in the paper by Paterek et al [33]

Overall, in terms of the discussion in Appendix 11  $\widehat{W}_{0L}$  would be *Charlie's* description of the initial state, whereas *Alice* would describe it as  $|\Psi\rangle_{0L} \langle\Psi|_{0L}$ . Presumably in the paper by Dowling et al [62] what is referred to as the "state of the laboratory" be Charlie's reference frame, and what they refer to as the "internal reference frame" would refer to that of Alice. However, whether Alice could actually prepare such a state as  $|\Psi\rangle_{0L} \langle\Psi|_{0L}$  is controversial - see SubSections 2.7 and 2.9, though here this is assumed to be possible.

### 12.1.4 Process - Alice and Charlie Descriptions

There are three stages in the process, the first being with the interaction that turns separate atoms A and B into the molecule AB turned on at Feshbach

resonance for a time  $t = \pi/(2\kappa < n >)$ , the second being free evolution at large Feshbach detuning  $\Delta$  for a time  $\tau$  leading to a phase factor  $\phi = \Delta\tau$ , the third being again with the interaction turned on at Feshbach resonance for a further time  $t = \pi/(2\kappa < n >)$ . The typical initial state  $|\Psi\rangle_{0L}$  given by  $|A\rangle|\beta\rangle$  (eq (11)) evolves into  $|\Psi\rangle_{3L}$  given by (see eq. (32) of paper)

$$|\Psi\rangle_{3L} = \left( \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) |\beta\rangle \quad (243)$$

using approximations set out in eqs (27), (28) of the paper that depend on  $< n >$  being large. Here  $|M\rangle$  is a state with one molecule AB. Thus it looks like a coherent superposition of an atom state  $|A\rangle$  and a molecule state  $|M\rangle$  has been prepared, the atom plus molecule system being disentangled from the BEC. *Alice* would describe the final state of the system as  $|\Psi\rangle_{3L} \langle\Psi|_{3L}$ , so from her point of view a coherent superposition of an atom and a molecule has been prepared.

However, for *Charlie* the *final state* of the system is described by a density operator  $\widehat{W}_{3L}$  which is reconstructed by applying the twirling operator to  $|\Psi\rangle_{3L} \langle\Psi|_{3L}$ . Noting that

$$\exp(-i\widehat{N}_{tot}\theta) |\Psi\rangle_{3L} = \left( \exp(-i\theta) \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(-2i\theta) \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) |\beta \exp(-i\theta)\rangle \quad (244)$$

and using

$$Tr_2(|\beta \exp(-i\theta)\rangle \langle\beta \exp(-i\theta)|) = \langle\beta \exp(-i\theta)|\beta \exp(-i\theta)\rangle = 1 \quad (245)$$

we see that Charlie's final reduced density operator for the *atom-molecule system* is

$$\begin{aligned} \widehat{\rho}_{A-M}(3) &= Tr_2 \widehat{W}_{3L} \\ &= Tr_2 \int \frac{d\theta}{2\pi} \exp(-i\widehat{N}_{tot}\theta) |\Psi\rangle_{3L} \langle\Psi|_{3L} \exp(+i\widehat{N}_{tot}\theta) \\ &= \int \frac{d\theta}{2\pi} \left( \exp(-i\theta) \sin\left(\frac{\phi}{2}\right) |A\rangle - \exp(-2i\theta) \exp(i \arg \beta) \cos\left(\frac{\phi}{2}\right) |M\rangle \right) \\ &\quad \times \left( \exp(+i\theta) \sin\left(\frac{\phi}{2}\right) \langle A| - \exp(+2i\theta) \exp(-i \arg \beta) \cos\left(\frac{\phi}{2}\right) \langle M| \right) \\ &= \sin^2\left(\frac{\phi}{2}\right) |A\rangle \langle A| + \cos^2\left(\frac{\phi}{2}\right) |M\rangle \langle M| \end{aligned} \quad (246)$$

Thus the coherence terms like  $|A\rangle \langle M|$  and  $|M\rangle \langle A|$  do not appear in the final density operator when the average over  $\theta$  (not  $\beta$ ) is carried out.

For Charlie the density operator for the atom and molecule is of course a statistical mixture of a state with one atom and no molecule and a state with no atom and one molecule. The authors of [62] actually point this out in the paragraph after eq (35) where (presumably for the case  $\phi = \pi/4$ ) it is stated “the

state is found to be ... an incoherent mixture of an atom and a molecule.”. The probabilities for detecting an atom A or a molecule AB are as in eq (33) of the paper. In terms of Charlie’s description, the density operator at the end of the preparation process does *not* signify the existence of a coherent superposition of an atom and a molecule, as the title to the paper might be taken to imply. The existence of such a coherent superposition would of course be present in Alice’s description, but it is Charlie’s (laboratory) description that is more relevant.

### 12.1.5 Coherence Effects Without SSR Violation

Note that *coherence effects* are still present since the atom or molecule detection probabilities depend on the phase  $\phi$  associated with the free evolution stage of the process. However, as in many other instances, the presence of coherence effects does not require the existence of *coherent superposition states* that violate the super-selection rule. The authors actually point this out in the paragraph after eq (35), where it is stated “we have clearly predicted the standard operational signature of coherence, namely Ramsey type fringes, but the coherence is not present in our mathematical description of the system.” What they are referring to is Charlie’s description of the final state - which indeed shows no such coherence, but the belief that coherent superposition states are needed to predict coherence effects is mistaken.

To drive this point home, the process can be treated with the initial state for the BEC being given as a Fock state  $|N\rangle$ . With the interaction being given as in Eq.(232) (eq (14) in the paper) the state vector is a simple linear combination of two terms

$$|\Psi(t)\rangle = A(t) |A\rangle |N\rangle + B(t) |M\rangle |N-1\rangle \quad (247)$$

This is of course an entangled state. Coupled equations for the two amplitudes  $A(t)$  and  $B(t)$  can easily be obtained and simple solutions obtained for stages where the Feshbach detuning is either zero or large. The state vector is continuous from one stage to the next, and the reduced density operator at the end of the three stage process for the atom plus molecule sub-system can be obtained. It is of the form

$$\begin{aligned} \hat{\rho}_{A-M}(3) &= Tr_2(|\Psi(3)\rangle \langle \Psi(3)|) \\ &= \sin^2(\frac{\phi}{2}) |A\rangle \langle A| + \cos^2(\frac{\phi}{2}) |M\rangle \langle M| \end{aligned} \quad (248)$$

which is of course a statistical mixture of a state with one atom and no molecule and a state with no atom and one molecule - and is exactly the same result as obtained in the paper by Dowling et al.[62]. Note that coherence effects in regard to the interferometric dependence on  $\phi$  for measurements on the final state has been found without invoking either the description of the BEC via Glauber coherent states or the presence of a coherent superposition of an atomic and a molecular state. The result can easily be extended for the case where the BEC is initially in a statistical mixture of Fock states with differing  $N$  occurring with

a probability  $P_N$ . Each initial state  $|A\rangle |N\rangle$  evolves as in Eq. (247). We then would have

$$\begin{aligned}
\hat{\rho}_{A-M}(3) &= \text{Tr}_2(\sum_N P_N |\Psi_N(3)\rangle \langle \Psi_N(3)|) \\
&= \sum_N P_N \left( \sin^2(\frac{\phi}{2}) |A\rangle \langle A| + \cos^2(\frac{\phi}{2}) |M\rangle \langle M| \right) \\
&= \sin^2(\frac{\phi}{2}) |A\rangle \langle A| + \cos^2(\frac{\phi}{2}) |M\rangle \langle M|
\end{aligned} \tag{249}$$

which is the same as before. Allowing for a statistical mixture of Fock states makes no difference to the interferometric result.

### 12.1.6 Conclusion

Dowling et al [62] state in their abstract that “we demonstrate that it is possible to perform a Ramsey-type interference experiment to exhibit a coherent superposition of a single atom and a diatomic molecule” . However the interferometric or coherence effects (involving the dependence on  $\phi$ ) cannot be said to exhibit the *existence* of such a coherent superposition, since the same interferometric results can be obtained *without* ever introducing such a quantum state. There is *not* a convincing case that quantum states that violate the super-selection rule forbidding the creation of coherent superpositions of Fock states with differing particle numbers can be *created*, even in Alice’s reference system. The fact that an SSR violating state  $|\Psi\rangle_{3L} \langle \Psi|_{3L}$  is created in Alice’s reference system is not surprising, because in the process considered the initial state  $|\beta\rangle$  for the BEC was assumed as a factor in Alice’s initial state, and this was itself inconsistent with the SSR. Furthermore, such SSR violating states are not *needed* to describe coherence and interference effects, so that justification for their physical existence also fails.

## 12.2 Detection of Coherent Superposition of a Vacuum and a One-Boson State ?

Whether such super-selection rule violating states can be detected has also not been justified. For example, consider the state given by a superposition of a one boson state and the vacuum state (as discussed in [63]). Consider an interferometric process in which one mode  $A$  for a two mode BEC interferometer is initially in the state  $\alpha |0\rangle + \beta |1\rangle$ , and the other mode  $B$  is initially in the state  $|0\rangle$  - thus  $|\Psi(i)\rangle = (\alpha |0\rangle + \beta |1\rangle)_A \otimes |0\rangle_B$  in the usual occupancy number notation, where  $|\alpha|^2 + |\beta|^2 = 1$ . Modes  $A, B$  could refer to two different hyperfine states of a bosonic atom with non-relativistic energies  $\hbar\omega_A$  and  $\hbar\omega_B$ , mode annihilation operators  $\hat{a}, \hat{b}$ . The modes are first coupled by a *beam splitter*, which could be a resonant microwave pulse that causes transitions between the two hyperfine



states and which can be described via a unitary operator  $\hat{U}_{BS}$  such that

$$\begin{aligned}\hat{U}_{BS}(|1\rangle_A \otimes |0\rangle_B) &= (|1\rangle_A \otimes |0\rangle_B - i|0\rangle_A \otimes |1\rangle_B)/\sqrt{2} \\ \hat{U}_{BS}(|0\rangle_A \otimes |1\rangle_B) &= (-i|1\rangle_A \otimes |0\rangle_B + |0\rangle_A \otimes |1\rangle_B)/\sqrt{2} \\ \hat{U}_{BS}(|0\rangle_A \otimes |0\rangle_B) &= (|0\rangle_A \otimes |0\rangle_B).\end{aligned}\quad (250)$$

After passing through the beam splitter the system is allowed to evolve freely for a time  $\tau$ , the Hamiltonian being  $\hat{H}_{free} = (mc^2 + \hbar\omega_A)\hat{a}^\dagger\hat{a} + (mc^2 + \hbar\omega_B)\hat{b}^\dagger\hat{b}$  - where collisional effects have been ignored and the rest mass energy included for completeness. Following the free evolution stage, the modes are then coupled again via a beam splitter, and the probability of an atom being found in modes  $A, B$  then being measured. A straightforward treatment of the evolution shows that the final state is given by

$$\begin{aligned}|\Psi(f)\rangle &= \alpha(|0\rangle_A \otimes |0\rangle_B) \\ &\quad + \beta \exp(-i\{mc^2/\hbar + \omega_A\}\tau) \\ &\quad \times \left( \frac{1 - \exp(-i\Delta\tau)}{2} (|1\rangle_A \otimes |0\rangle_B) - i \frac{1 + \exp(-i\Delta\tau)}{2} (|0\rangle_A \otimes |1\rangle_B) \right)\end{aligned}\quad (251)$$

where  $\Delta = \omega_B - \omega_A$  is the detuning. The probabilities of finding one atom in modes  $A, B$  respectively are

$$P_{10} = |\beta|^2 \sin^2(\Delta\tau/2) \quad P_{01} = |\beta|^2 \cos^2(\Delta\tau/2) \quad (252)$$

Thus whilst coherence effects occur depending on the phase difference  $\phi = \Delta\tau$  associated with the interferometric process, the overall detection probabilities only depend on the initial state via  $|\beta|^2$ . There is no dependence on the *relative phase* between  $\alpha$  and  $\beta$ , as would be required if the superposition state  $\alpha|0\rangle + \beta|1\rangle$  is to be specified from the measurement results. Exactly the same detection probabilities are obtained if the initial state is the mixed state  $\hat{\rho}(i) = |\alpha|^2(|0\rangle_A \langle 0|_A \otimes |0\rangle_B \langle 0|_B) + |\beta|^2(|1\rangle_A \langle 1|_A \otimes |0\rangle_B \langle 0|_B)$ , in which the vacuum state for mode  $A$  occurs with a probability  $|\alpha|^2$  and the one boson state for mode  $A$  occurs with a probability  $|\beta|^2$ . In this example the coherent superposition associated with the super-selection rule violating state would not be detected in the interferometric process. The paper by Dunningham et al [63] considers first a detection process that involves using a Glauber coherent state as one of the input states. Similar interference effects as in Eq. (252) are obtained. A second detection process in which the single term Glauber coherent state is replaced by a statistical mixture with all phases equally weighted is considered next, leading to the same interference effects. This again confirms that it is not necessary to invoke the existence of coherent superpositions of number states in order to demonstrate interference effects.

## 13 Appendix 5 - Non-Physical Two Mode States

We now consider some possible states for the second mode  $B$  - to be combined with  $\hat{\rho}_1^A$ ,  $\hat{\rho}_2^A$  and  $P_1$ ,  $P_2$  as in Eq. (42). These states are two general pure orthogonal states of the form  $\alpha|0\rangle_B + \beta|1\rangle_B$  and  $-\beta^*|0\rangle_B + \alpha^*|1\rangle_B$  with  $(|\alpha|^2 + |\beta|^2) = 1$ . We have

$$\begin{aligned}\hat{\rho}_1^B &= ((\alpha|0\rangle_B + \beta|1\rangle_B))((\alpha^*\langle 0|_B + \beta^*\langle 1|_B)) \\ \hat{\rho}_2^B &= ((-\beta^*|0\rangle_B + \alpha^*|1\rangle_B))((-\beta\langle 0|_B + \alpha\langle 1|_B))\end{aligned}\quad (253)$$

This gives the reduced density operator

$$\hat{\rho}_B = \frac{1}{2}(|0\rangle_B\langle 0|_B) + \frac{1}{2}(|1\rangle_B\langle 1|_B) \quad (254)$$

A straightforward calculation gives for the overall density operator for the two mode non-entangled state as in Eq. (1)

$$\hat{\rho} = \hat{\rho}_1 + \hat{\rho}_2$$

where the  $\hat{\rho}_1$ ,  $\hat{\rho}_2$  are contributions that are consistent with or inconsistent with the super-selection rule. We have

$$\begin{aligned}\hat{\rho}_1 &= \frac{1}{4}|0\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 0|_B + \frac{1}{4}|1\rangle_A\langle 1|_A \otimes |0\rangle_B\langle 0|_B \\ &+ \frac{1}{4}|0\rangle_A\langle 0|_A \otimes |1\rangle_B\langle 1|_B + \frac{1}{4}|1\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B \\ &+ \frac{1}{2}\alpha^*\beta|0\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 0|_B + \frac{1}{2}\alpha\beta^*|1\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 1|_B\end{aligned}\quad (255)$$

and

$$\begin{aligned}\hat{\rho}_2 &= \frac{1}{4}(|\alpha|^2 - |\beta|^2)|0\rangle_A\langle 1|_A \otimes |0\rangle_B\langle 0|_B + \frac{1}{4}(|\alpha|^2 - |\beta|^2)|1\rangle_A\langle 0|_A \otimes |0\rangle_B\langle 0|_B \\ &+ \frac{1}{4}(|\beta|^2 - |\alpha|^2)|0\rangle_A\langle 1|_A \otimes |1\rangle_B\langle 1|_B + \frac{1}{4}(|\beta|^2 - |\alpha|^2)|1\rangle_A\langle 0|_A \otimes |1\rangle_B\langle 1|_B \\ &+ \frac{1}{2}\alpha^*\beta|1\rangle_A\langle 0|_A \otimes |1\rangle_B\langle 0|_B + \frac{1}{2}\alpha\beta^*|0\rangle_A\langle 1|_A \otimes |0\rangle_B\langle 1|_B\end{aligned}\quad (256)$$

Now to make  $\hat{\rho}_2 = 0$  requires  $|\alpha|^2 = |\beta|^2$  so that the first four terms in  $\hat{\rho}_2$  are zero. This in combination with  $|\alpha|^2 + |\beta|^2 = 1$  leads to  $|\alpha| = |\beta| = \frac{1}{\sqrt{2}}$ . However this results in the remaining two terms in  $\hat{\rho}_2$  - which are coherences between  $N = 0$  and  $N = 2$  states - always being non-zero. Overall then, no choice of  $\alpha$ ,  $\beta$  will lead to a overall density operator which is physical. Adding further states  $|2\rangle_B$ ,  $|3\rangle_B$ , ...does not rectify the problem.

## 14 Appendix 6 - Derivation of Sorensen et al Results

Sorensen et al [41] derive a number of inequalities from which they deduce a further inequality for the spin squeezing parameter in the case of a non-entangled state. From this result they conclude that spin squeezing implies entanglement. The final inequality they obtain for a non-entangled state is

$$\langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right) \quad (257)$$

Their approach is based on writing the density operator for a non-entangled state of  $N$  identical particles as in Eq. (24)

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes \dots = \sum_R P_R \hat{\rho}_R \quad (258)$$

The spin operators are defined as  $\hat{S}_x = \sum_i \hat{S}_x^i = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| + |\phi_a(i)\rangle \langle \phi_b(i)|)/2$ ;  $\hat{S}_y = \sum_i \hat{S}_y^i = \sum_i (|\phi_b(i)\rangle \langle \phi_a(i)| - |\phi_a(i)\rangle \langle \phi_b(i)|)/2i$ ;  $\hat{S}_z = \sum_i \hat{S}_z^i = \sum_i (|\phi_b(i)\rangle \langle \phi_b(i)| - |\phi_a(i)\rangle \langle \phi_a(i)|)/2$ , where the sum  $i$  is over the identical atoms and each atom is associated with two states  $|\phi_a\rangle$  and  $|\phi_b\rangle$ . Clearly, the spin operators satisfy the standard commutation rules for angular momentum operators.

Sorensen et al [41] state that the variance for  $\hat{S}_z$  satisfies the result

$$\langle \Delta \hat{S}_z^2 \rangle = \frac{N}{4} - \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R^2 + \sum_R P_R \langle \hat{S}_z \rangle_R^2 - \langle \hat{S}_z \rangle^2 \quad (259)$$

To prove this we have

$$\begin{aligned} \langle \hat{S}_z^2 \rangle &= \sum_R P_R \text{Tr}(\hat{\rho}_R \sum_i \sum_j \hat{S}_z^i \hat{S}_z^j) \\ &= \sum_R P_R \left( \sum_i \langle (\hat{S}_z^i)^2 \rangle_R + \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right) \\ &= \frac{N}{4} + \sum_R P_R \left( \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right) \end{aligned} \quad (260)$$

where we have used

$$\begin{aligned} (\hat{S}_z^i)^2 &= \frac{1}{4} (|\phi_b(i)\rangle \langle \phi_b(i)| - |\phi_a(i)\rangle \langle \phi_a(i)|)^2 \\ &= \frac{1}{4} (|\phi_b(i)\rangle \langle \phi_b(i)| \phi_b(i)\rangle \langle \phi_b(i)| - (|\phi_b(i)\rangle \langle \phi_b(i)| \phi_a(i)\rangle \langle \phi_a(i)|) \\ &\quad + \frac{1}{4} (-(|\phi_a(i)\rangle \langle \phi_a(i)| \phi_b(i)\rangle \langle \phi_b(i)| + (|\phi_a(i)\rangle \langle \phi_a(i)| \phi_a(i)\rangle \langle \phi_a(i)|)) \\ &= \frac{1}{4} ((|\phi_b(i)\rangle \langle \phi_b(i)| + (|\phi_a(i)\rangle \langle \phi_a(i)|)) \\ &= \frac{1}{4} \hat{1}_i \end{aligned} \quad (261)$$

a result based on the orthogonality, normalisation and completeness of the states  $|\phi_a(i)\rangle, |\phi_b(i)\rangle$ . Also

$$\begin{aligned}\langle \hat{S}_z \rangle_R &= \text{Tr}(\hat{\rho}_R \sum_i \hat{S}_z^i) \\ &= \sum_i \langle \hat{S}_z^i \rangle_R \\ \sum_R P_R \langle \hat{S}_z \rangle_R^2 &= \sum_R P_R \left( \sum_i \langle \hat{S}_z^i \rangle_R^2 + \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right)\end{aligned}\quad (262)$$

so eliminating the term  $\sum_R P_R \left( \sum_{i \neq j} \langle \hat{S}_z^i \rangle_R \langle \hat{S}_z^j \rangle_R \right)$  gives the required expression for  $\langle \Delta \hat{S}_z^2 \rangle = \langle \hat{S}_z^2 \rangle - \langle \hat{S}_z \rangle^2$ .

Next, Sorensen et al [41] state that

$$\langle \hat{S}_x \rangle^2 \leq N \sum_R P_R \sum_i \langle \hat{S}_x^i \rangle_R^2 \quad \langle \hat{S}_y \rangle^2 \leq N \sum_R P_R \sum_i |\langle \hat{S}_y^i \rangle_R|^2 \quad (263)$$

To prove this we have

$$\begin{aligned}\langle \hat{S}_x \rangle &= \sum_R P_R \text{Tr}(\hat{\rho}_R \sum_i \hat{S}_x^i) \\ &= \sum_R P_R \sum_i \langle \hat{S}_x^i \rangle_R \\ |\langle \hat{S}_x \rangle| &\leq \sum_R P_R \sum_i |\langle \hat{S}_x^i \rangle_R|\end{aligned}\quad (264)$$

since the modulus of a sum is less than or equal to the sum of the moduli. Now

$$\begin{aligned}\langle \hat{S}_x \rangle^2 &= |\langle \hat{S}_x \rangle|^2 \leq \left( \sum_R P_R \sum_i |\langle \hat{S}_x^i \rangle_R| \right)^2 \\ &\leq \sum_R P_R \left( \sum_i |\langle \hat{S}_x^i \rangle_R| \right)^2\end{aligned}\quad (265)$$

using the general result that  $\left( \sum_R P_R \sqrt{C_R} \right)^2 \leq \sum_R P_R C_R$ , where  $\sum_R P_R = 1$  with here  $\sqrt{C_R} = \sum_i |\langle \hat{S}_x^i \rangle_R|$ . Next consider

$$\begin{aligned}y &= N \sum_i |\langle \hat{S}_x^i \rangle_R|^2 \\ z &= \left( \sum_i |\langle \hat{S}_x^i \rangle_R| \right)^2 = \left( \sum_i |\langle \hat{S}_x^i \rangle_R| \right)^2 \\ y - z &= \sum_{i < j} (|\langle \hat{S}_x^i \rangle_R| - |\langle \hat{S}_x^j \rangle_R|)^2 \geq 0\end{aligned}\quad (266)$$

so that

$$\langle \hat{S}_x \rangle^2 \leq N \sum_R P_R \sum_i |\langle \hat{S}_x^i \rangle_R|^2 \quad \langle \hat{S}_y \rangle^2 \leq N \sum_R P_R \sum_i |\langle \hat{S}_y^i \rangle_R|^2 \quad (267)$$

which is the required result. The inequality for  $\langle \hat{S}_y \rangle^2$  is proved similarly.

Another inequality is stated [41] for  $\langle \hat{S}_z \rangle^2$ . This is

$$\langle \hat{S}_z \rangle^2 \leq \sum_R P_R \langle \hat{S}_z \rangle_R^2 \quad (268)$$

To show this we have

$$\begin{aligned} \langle \hat{S}_z \rangle &= \sum_R P_R \text{Tr}(\hat{\rho}_R \sum_i \hat{S}_z^i) \\ &= \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R \\ &= \sum_R P_R \langle \hat{S}_z \rangle_R \\ |\langle \hat{S}_z \rangle| &\leq \sum_R P_R |\langle \hat{S}_z \rangle_R| \end{aligned} \quad (269)$$

so that

$$\begin{aligned} \langle \hat{S}_z \rangle^2 &= |\langle \hat{S}_z \rangle|^2 \leq \left( \sum_R P_R |\langle \hat{S}_z \rangle_R| \right)^2 \\ &\leq \sum_R P_R |\langle \hat{S}_z \rangle_R|^2 \\ &= \sum_R P_R \langle \hat{S}_z \rangle_R^2 \end{aligned} \quad (270)$$

using the general result that  $\left( \sum_R P_R \sqrt{C_R} \right)^2 \leq \sum_R P_R C_R$ , where  $\sum_R P_R = 1$  with

here  $\sqrt{C_R} = |\langle \hat{S}_z \rangle_R|$ .

Finally, we find that

$$\begin{aligned} \sum_R P_R \sum_i \left( \langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 \right) &\leq \frac{1}{4} N \\ - \sum_R P_R \sum_i \left( \langle \hat{S}_z^i \rangle_R^2 \right) &\geq -\frac{1}{4} N + \sum_R P_R \sum_i \left( \langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 \right) \end{aligned} \quad (271)$$

To show this we use the properties of the density operator  $\hat{\rho}_R^i$  for the  $i$ th particle of Hermitiancy, positiveness, unit trace  $Tr(\hat{\rho}_R^i) = 1$  and  $Tr(\hat{\rho}_R^i)^2 \leq 1$ . In terms of matrix elements of the density operator  $\hat{\rho}_R^i$  between the two states  $|\phi_a(i)\rangle$ ,  $|\phi_b(i)\rangle$  the quantities  $\langle \hat{S}_x^i \rangle_R$ ,  $\langle \hat{S}_y^i \rangle_R$  and  $\langle \hat{S}_z^i \rangle_R$  are

$$\begin{aligned}\langle \hat{S}_x^i \rangle_R &= Tr(\hat{\rho}_R^i \frac{1}{2}(|\phi_b(i)\rangle \langle \phi_a(i)| + |\phi_a(i)\rangle \langle \phi_b(i)|)) \\ &= \frac{1}{2} (\rho_{ab}^i + \rho_{ba}^i) \\ \langle \hat{S}_y^i \rangle_R &= \frac{1}{2i} (\rho_{ab}^i - \rho_{ba}^i) \\ \langle \hat{S}_z^i \rangle_R &= \frac{1}{2} (\rho_{bb}^i - \rho_{aa}^i)\end{aligned}\tag{272}$$

where  $\rho_{cd}^i = \langle \phi_c(i) | \hat{\rho}_R^i | \phi_d(i) \rangle$ . The Hermitiancy and positiveness of  $\hat{\rho}_R^i$  show that  $\rho_{bb}^i$  and  $\rho_{aa}^i$  are real and positive,  $\rho_{ab}^i = (\rho_{ba}^i)^*$  and  $\rho_{aa}^i \rho_{bb}^i - |\rho_{ab}^i|^2 \geq 0$ . The condition  $Tr(\hat{\rho}_R^i) = 1$  leads to  $\rho_{aa}^i + \rho_{bb}^i = 1$ , from which  $Tr(\hat{\rho}_R^i)^2 \leq 1$  follows using the previous positivity results. Taken together these conditions lead to the following useful parametrisation of the density matrix elements

$$\begin{aligned}\rho_{aa}^i &= \sin^2 \alpha_i & \rho_{bb}^i &= \cos^2 \alpha_i \\ \rho_{ab}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \sin^2 \beta_i \exp(+i\phi_i) & \rho_{ba}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \sin^2 \beta_i \exp(-i\phi_i)\end{aligned}\tag{273}$$

where  $\alpha_i$ ,  $\beta_i$  and  $\phi_i$  are real. In terms of these quantities we then have

$$\begin{aligned}\langle \hat{S}_x^i \rangle_R &= \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \cos \phi_i \\ \langle \hat{S}_y^i \rangle_R &= \frac{1}{2} \sin 2\alpha_i \sin^2 \beta_i \sin \phi_i \\ \langle \hat{S}_z^i \rangle_R &= \frac{1}{2} \cos 2\alpha_i\end{aligned}\tag{274}$$

It is then easy to show that

$$\begin{aligned}\langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 &= \frac{1}{4} - \frac{1}{4} \sin^2 2\alpha_i (1 - \sin^4 \beta_i) \\ &\leq \frac{1}{4}\end{aligned}\tag{275}$$

and the final inequality (271) then follows by taking the sum over particles  $i$  and then using  $\sum_R P_R = 1$ . If only the Schwarz inequality is used instead of the more detailed consequences of Hermitiancy, positiveness etc it can be shown that  $\langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 + \langle \hat{S}_z^i \rangle_R^2 \leq \frac{3}{4}$ , which though correct is not useful.

Combining the inequalities in Eqs. (263), (268) and (271) into Eq. (259)

shows that

$$\begin{aligned}
\langle \Delta \hat{S}_z^2 \rangle &= \frac{N}{4} - \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R^2 + \sum_R P_R \langle \hat{S}_z \rangle_R^2 - \langle \hat{S}_z \rangle^2 \\
&\geq \frac{N}{4} - \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R^2 \\
&\geq \frac{N}{4} - \frac{1}{4}N + \sum_R P_R \sum_i \left( \langle \hat{S}_x^i \rangle_R^2 + \langle \hat{S}_y^i \rangle_R^2 \right) \\
&\geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right)
\end{aligned} \tag{276}$$

for the case of a non-entangled state. This result is that in Sorensen et al.[41].

## 15 Appendix 7 - Revised Sorensen et al

### 15.1 Variance $\langle \Delta \hat{S}_x^2 \rangle$

Here we will see if the modified approach to Sorensen et al can lead to a useful inequality for  $\langle \Delta \hat{S}_x^2 \rangle$  or  $\langle \Delta \hat{S}_y^2 \rangle$  that applies when non-entangled states are those when *all* the separate modes  $\hat{a}_i$  and  $\hat{b}_i$  are the sub-systems . We will attempt to follow the approach used for the simple two mode case in Section 4.

Firstly, the *variance* for a Hermitian operator  $\hat{\Omega}$  in a mixed state

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R \quad (277)$$

is always greater than or equal to the the average of the variances for the separate components

$$\langle \Delta \hat{\Omega}^2 \rangle \geq \sum_R P_R \langle \Delta \hat{\Omega}^2 \rangle_R \quad (278)$$

where  $\langle \Delta \hat{\Omega}^2 \rangle = \text{Tr}(\hat{\rho} \Delta \hat{\Omega}^2)$  with  $\Delta \hat{\Omega} = \hat{\Omega} - \langle \hat{\Omega} \rangle$  and  $\langle \Delta \hat{\Omega}^2 \rangle_R = \text{Tr}(\hat{\rho}_R \Delta \hat{\Omega}_R^2)$  with  $\Delta \hat{\Omega}_R = \hat{\Omega} - \langle \hat{\Omega} \rangle_R$  . The proof is straight-forward and given in Ref. [69].

Next we calculate  $\langle \Delta \hat{S}_x^2 \rangle_R$ ,  $\langle \Delta \hat{S}_y^2 \rangle_R$  and  $\langle \hat{S}_x \rangle_R$ ,  $\langle \hat{S}_y \rangle_R$ ,  $\langle \hat{S}_z \rangle_R$  for the case where

$$\hat{\rho} = \sum_R P_R \left( \hat{\rho}_R^{a1} \otimes \hat{\rho}_R^{b1} \right) \otimes \left( \hat{\rho}_R^{a2} \otimes \hat{\rho}_R^{b2} \right) \otimes \left( \hat{\rho}_R^{a3} \otimes \hat{\rho}_R^{b3} \right) \otimes \dots \quad (279)$$

as is required for a *general non-entangled* state *all*  $2N$  modes. Furthermore, the density operators for the individual modes must represent possible physical states for such modes, so the super-selection rule for atom number applies and we have

$$\begin{aligned} \langle (\hat{a}_i)^n \rangle_{a_i} &= \text{Tr}(\hat{\rho}_R^{a i} (\hat{a}_i)^n) = 0 & \langle (\hat{a}_i^\dagger)^n \rangle_{a_i} &= \text{Tr}(\hat{\rho}_R^{a i} (\hat{a}_i^\dagger)^n) = 0 \\ \langle (\hat{b}_i)^m \rangle_{b_i} &= \text{Tr}(\hat{\rho}_R^{b i} (\hat{b}_i)^m) = 0 & \langle (\hat{b}_i^\dagger)^m \rangle_{b_i} &= \text{Tr}(\hat{\rho}_R^{b i} (\hat{b}_i^\dagger)^m) = 0 \end{aligned} \quad (280)$$

The Schwinger spin operators are

$$\begin{aligned} \hat{S}_x &= \sum_i (\hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i)/2 = \sum_i \hat{S}_x^i \\ \hat{S}_y &= \sum_i (\hat{b}_i^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{b}_i)/2i = \sum_i \hat{S}_y^i \\ \hat{S}_z &= \sum_i (\hat{b}_i^\dagger \hat{b}_i - \hat{a}_i^\dagger \hat{a}_i)/2 = \sum_i \hat{S}_z^i \end{aligned} \quad (281)$$



where  $\hat{a}_i$ ,  $\hat{b}_i$  and  $\hat{a}_i^\dagger$ ,  $\hat{b}_i^\dagger$  respectively are mode annihilation, creation operators. From Eqs. (281) we find that

$$\hat{S}_x^2 = \sum_i (\hat{S}_x^i)^2 + \sum_{i \neq j} \hat{S}_x^i \hat{S}_x^j \quad (282)$$

so that on taking the trace with  $\hat{\rho}_R$  and using Eqs. (279) we get after applying the commutation rules  $[\hat{e}, \hat{e}^\dagger] = \hat{1}$  ( $\hat{e} = \hat{a}$  or  $\hat{b}$ )

$$\langle \hat{S}_x^2 \rangle_R = \sum_i \langle (\hat{S}_x^i)^2 \rangle_R + \sum_{i \neq j} \langle \hat{S}_x^i \rangle_R \langle \hat{S}_x^j \rangle_R \quad (283)$$

As we also have

$$\langle \hat{S}_x \rangle_R = \sum_i \langle \hat{S}_x^i \rangle_R \quad \langle \hat{S}_x \rangle_R^2 = \sum_i \langle \hat{S}_x^i \rangle_R^2 + \sum_{i \neq j} \langle \hat{S}_x^i \rangle_R \langle \hat{S}_x^j \rangle_R \quad (284)$$

using Eqs. (279) and we see finally that the variance  $\langle \Delta \hat{S}_x^2 \rangle_R$  is

$$\langle \Delta \hat{S}_x^2 \rangle_R = \sum_i \langle (\hat{S}_x^i)^2 \rangle_R - \sum_i \langle \hat{S}_x^i \rangle_R^2 \quad (285)$$

all the terms with  $i \neq j$  cancelling out. and therefore from Eq. (278)

$$\langle \Delta \hat{S}_x^2 \rangle \geq \sum_R P_R \sum_i \left( \langle (\hat{S}_x^i)^2 \rangle_R - \langle \hat{S}_x^i \rangle_R^2 \right) \quad (286)$$

But using (280)

$$\begin{aligned} (\hat{S}_x^i)^2 &= \frac{1}{4} (\hat{b}_i^\dagger \hat{a}_i \hat{b}_i^\dagger \hat{a}_i + \hat{b}_i^\dagger \hat{a}_i \hat{a}_i^\dagger \hat{b}_i + \hat{a}_i^\dagger \hat{b}_i \hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i \hat{a}_i^\dagger \hat{b}_i) \\ \langle (\hat{S}_x^i)^2 \rangle_R &= \frac{1}{4} (\langle (\hat{b}^\dagger \hat{b})_i \rangle_R + \langle (\hat{a}^\dagger \hat{a})_i \rangle_R + \frac{1}{2} (\langle (\hat{a}^\dagger \hat{a})_i \rangle_R \langle (\hat{b}^\dagger \hat{b})_i \rangle_R)) \end{aligned} \quad (287)$$

and

$$\langle \hat{S}_x^i \rangle_R = 0 \quad (288)$$

so that

$$\langle \Delta \hat{S}_x^2 \rangle \geq \sum_R P_R \sum_i \left( \frac{1}{4} (\langle (\hat{b}^\dagger \hat{b})_i \rangle_R + \langle (\hat{a}^\dagger \hat{a})_i \rangle_R + \frac{1}{2} (\langle (\hat{a}^\dagger \hat{a})_i \rangle_R \langle (\hat{b}^\dagger \hat{b})_i \rangle_R)) \right) \quad (289)$$

Now using (280)

$$\langle \hat{S}_z^i \rangle_R = \frac{1}{2} (\langle (\hat{b}^\dagger \hat{b})_i \rangle_R - \langle (\hat{a}^\dagger \hat{a})_i \rangle_R) \quad (290)$$

$$\begin{aligned}
\langle \hat{S}_z \rangle &= \sum_R P_R \sum_i \langle \hat{S}_z^i \rangle_R \\
\frac{1}{2} |\langle \hat{S}_z \rangle| &= \frac{1}{2} \sum_R P_R \left| \sum_i \frac{1}{2} (\langle \hat{b}^\dagger \hat{b} \rangle_R - \langle \hat{a}^\dagger \hat{a} \rangle_R) \right| \\
&\leq \sum_R P_R \frac{1}{4} \sum_i |\langle \hat{b}^\dagger \hat{b} \rangle_R - \langle \hat{a}^\dagger \hat{a} \rangle_R| \\
&\leq \sum_R P_R \frac{1}{4} \sum_i (\langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R) \tag{291}
\end{aligned}$$

and thus

$$\begin{aligned}
&\langle \Delta \hat{S}_x^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| \\
&\geq \sum_R P_R \sum_i \left( \frac{1}{4} (\langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R) + \frac{1}{2} (\langle \hat{a}^\dagger \hat{a} \rangle_R \langle \hat{b}^\dagger \hat{b} \rangle_R) \right) \\
&\quad - \sum_R P_R \frac{1}{4} \sum_i (\langle \hat{b}^\dagger \hat{b} \rangle_R + \langle \hat{a}^\dagger \hat{a} \rangle_R) \\
&= \sum_R P_R \frac{1}{2} \sum_i (\langle \hat{a}^\dagger \hat{a} \rangle_R \langle \hat{b}^\dagger \hat{b} \rangle_R) \\
&\geq 0 \tag{292}
\end{aligned}$$

A similar proof shows that  $\langle \Delta \hat{S}_y^2 \rangle - \frac{1}{2} |\langle \hat{S}_z \rangle| \geq 0$  for the non-entangled state of all  $2N$  modes.

This shows that for the general non-entangled state with all modes  $\hat{a}_i$  and  $\hat{b}_i$  as the sub-systems, the variances for two of the spin fluctuations  $\langle \Delta \hat{S}_x^2 \rangle$  and  $\langle \Delta \hat{S}_y^2 \rangle$  are both greater than  $\frac{1}{2} |\langle \hat{S}_z \rangle|$ , and hence there is no spin squeezing for  $\hat{S}_x$  or  $\hat{S}_y$ . Note that as  $|\langle \hat{S}_y \rangle| = 0$ , the quantity  $\sqrt{(|\langle \hat{S}_{\perp 1} \rangle|^2 + |\langle \hat{S}_{\perp 2} \rangle|^2)}$  is the same as  $|\langle \hat{S}_z \rangle|$ , so the alternative criterion in Eq. (64) is the same as that in Eq. (60) which is used here.

For the other spin fluctuation  $\langle \Delta \hat{S}_z^2 \rangle$  since we have

$$\langle \hat{S}_x \rangle = \sum_R P_R \langle \hat{S}_x \rangle_R = 0 \quad \langle \hat{S}_y \rangle = \sum_R P_R \langle \hat{S}_y \rangle_R = 0 \tag{293}$$

then the other two uncertainty relationships just give  $\langle \Delta \hat{S}_y^2 \rangle \langle \Delta \hat{S}_z^2 \rangle \geq 0$ ;  $\langle \Delta \hat{S}_z^2 \rangle \langle \Delta \hat{S}_x^2 \rangle \geq 0$ , so spin squeezing in  $\hat{S}_z$  is meaningless.

Hence we have shown that for a *non-entangled* physical state for all the  $2N$  modes  $\hat{a}_i$  and  $\hat{b}_i$

$$\langle \Delta \hat{S}_x^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle| \quad \text{and} \quad \langle \Delta \hat{S}_y^2 \rangle \geq \frac{1}{2} |\langle \hat{S}_z \rangle| \tag{294}$$

so that spin squeezing in either  $\hat{S}_x$  or  $\hat{S}_y$  requires entanglement.

## 15.2 Variance $\langle \Delta \hat{S}_z^2 \rangle$

Here we will see if the modified approach to Sorensen et al can lead to a useful inequality for  $\langle \Delta \hat{S}_z^2 \rangle$  that applies when non-entangled states are those when the *pairs* of modes  $\hat{a}_i$  and  $\hat{b}_i$  are the separate sub-systems. We will attempt to follow the approach used by Sorensen et al when identical particles  $i$  were regarded as the sub-systems.

Now the general non-entangled state will be

$$\hat{\rho} = \sum_R P_R \hat{\rho}_R^1 \otimes \hat{\rho}_R^2 \otimes \hat{\rho}_R^3 \otimes \dots \quad (295)$$

where the  $\hat{\rho}_R^i$  are now of the form given in Eq. (157) and the conditions in Eq. (280) no longer apply. The Fock states are of the form  $|N_{ia}\rangle \otimes |N_{ib}\rangle$  for the pair of modes  $\hat{a}_i$  and  $\hat{b}_i$ , and for this Fock state the total occupancy of the pair of modes is  $N_i = N_{ia} + N_{ib}$ . From the super-selection rule the density operator  $\hat{\rho}_R^i$  for the  $i$ th pair of modes  $\hat{a}_i$  and  $\hat{b}_i$  is diagonal in the total occupancy. For  $N_i = 0$  there is one non zero matrix element ( $\langle 0|_{ia} \otimes \langle 0|_{ib} \rangle \hat{\rho}_R^i (|0\rangle_{ia} \otimes |0\rangle_{ib})$ ). For  $N_i = 1$  there are four non zero matrix elements, which may be written

$$\begin{aligned} \langle \langle 1|_{ia} \otimes \langle 0|_{ib} \rangle \hat{\rho}_R^i (|1\rangle_{ia} \otimes |0\rangle_{ib}) &= \rho_{aa}^i \\ \langle \langle 1|_{ia} \otimes \langle 0|_{ib} \rangle \hat{\rho}_R^i (|0\rangle_{ia} \otimes |1\rangle_{ib}) &= \rho_{ab}^i \\ \langle \langle 0|_{ia} \otimes \langle 1|_{ib} \rangle \hat{\rho}_R^i (|1\rangle_{ia} \otimes |0\rangle_{ib}) &= \rho_{ba}^i \\ \langle \langle 0|_{ia} \otimes \langle 1|_{ib} \rangle \hat{\rho}_R^i (|0\rangle_{ia} \otimes |1\rangle_{ib}) &= \rho_{bb}^i \end{aligned} \quad (296)$$

For  $N_i = 2$  there are nine non zero matrix element ( $\langle \langle 2|_{ia} \otimes \langle 0|_{ib} \rangle \hat{\rho}_R^i (|2\rangle_{ia} \otimes |0\rangle_{ib})$ , ..., ( $\langle \langle 0|_{ia} \otimes \langle 2|_{ib} \rangle \hat{\rho}_R^i (|0\rangle_{ia} \otimes |2\rangle_{ib})$ ) and the number increases with  $N_i$ .

If we restrict ourselves to general entangled states where  $N_i = 1$  for all pairs of modes, then the density operator  $\hat{\rho}_R^i$  is of then form

$$\begin{aligned} \hat{\rho}_R^i &= \rho_{aa}^i (|1\rangle_{ia} \langle 1|_{ia} \otimes |0\rangle_{ib} \langle 0|_{ib}) + \rho_{ab}^i (|1\rangle_{ia} \langle 0|_{ia} \otimes |0\rangle_{ib} \langle 1|_{ib}) \\ &\quad + \rho_{ba}^i (|0\rangle_{ia} \langle 1|_{ia} \otimes |1\rangle_{ib} \langle 0|_{ib}) + \rho_{bb}^i (|0\rangle_{ia} \langle 0|_{ia} \otimes |1\rangle_{ib} \langle 1|_{ib}) \end{aligned} \quad (297)$$

In addition Hermitiancy, positivity, unit trace  $Tr(\hat{\rho}_R^i) = 1$  and  $Tr(\hat{\rho}_R^i)^2 \leq 1$  can be used as in Eq (273) to parameterise the matrix elements in (296).

$$\begin{aligned} \rho_{aa}^i &= \sin^2 \alpha_i & \rho_{bb}^i &= \cos^2 \alpha_i \\ \rho_{ab}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \sin^2 \beta_i \exp(+i\phi_i) & \rho_{ba}^i &= \sqrt{\sin^2 \alpha_i \cos^2 \alpha_i} \sin^2 \beta_i \exp(-i\phi_i) \end{aligned} \quad (298)$$

The expectation values for the spin operators  $\hat{S}_x^i$ ,  $\hat{S}_y^i$  and  $\hat{S}_z^i$  associated with the  $i$ th pair of modes are then

$$\begin{aligned}
\langle \hat{S}_x^i \rangle_R &= \text{Tr}(\hat{\rho}_R^i \frac{1}{2}(\hat{b}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{b}_i)) \\
&= \frac{1}{2} (\rho_{ab}^i + \rho_{ba}^i) \\
\langle \hat{S}_y^i \rangle_R &= \frac{1}{2i} (\rho_{ab}^i - \rho_{ba}^i) \\
\langle \hat{S}_z^i \rangle_R &= \frac{1}{2} (\rho_{bb}^i - \rho_{aa}^i)
\end{aligned} \tag{299}$$

which are of exactly the same form as in Eq. (272) as in the Appendix 14 derivation of the original Sorensen et al [41] results based on treating identical particles as the sub-systems. The proof however is now different and rests on restricting the states  $\hat{\rho}_R^i$  to each containing exactly one boson.

The remainder of the proof is exactly the same as in Appendix 14 and we find that

$$\langle \Delta \hat{S}_z^2 \rangle \geq \frac{1}{N} \left( \langle \hat{S}_x \rangle^2 + \langle \hat{S}_y \rangle^2 \right) \tag{300}$$

for non-entangled *pairs* of modes  $\hat{a}_i$  and  $\hat{b}_i$ . Thus when the interpretation is changed so that are the separate sub-systems are these pairs of modes, it follows that spin squeezing requires entanglement of all the mode pairs.

## 16 Appendix 8 - Heisenberg Uncertainty Principle Results

Here we derive the results in SubSection 5.4 leading to inequalities for the variance  $\langle \Delta \hat{J}_x^2 \rangle$  considered as a function of  $|\langle \hat{J}_z \rangle|$  for states where the spin operators are chosen such that  $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$ .

From the Schwarz inequality  $\langle \hat{J}_z \rangle^2 \leq \langle \hat{J}_z^2 \rangle$  so that

$$\langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle + \langle \hat{J}_z \rangle^2 \leq \langle \hat{J}_x^2 \rangle + \langle \hat{J}_y^2 \rangle + \langle \hat{J}_z^2 \rangle = J(J+1) \quad (301)$$

giving Eq. (169). Subtracting  $\langle \hat{J}_x \rangle^2 = \langle \hat{J}_y \rangle^2 = 0$  from each side gives

$$\langle \Delta \hat{J}_x^2 \rangle + \langle \Delta \hat{J}_y^2 \rangle + \langle \hat{J}_z \rangle^2 \leq J(J+1) \quad (302)$$

Substituting for  $\langle \Delta \hat{J}_y^2 \rangle$  from the Heisenberg uncertainty principle result in Eq. (170) gives

$$\langle \Delta \hat{J}_x^2 \rangle^2 - \left( J(J+1) - \langle \hat{J}_z \rangle^2 \right) \langle \Delta \hat{J}_x^2 \rangle + \frac{1}{4} \xi \langle \hat{J}_z \rangle^2 \leq 0 \quad (303)$$

The left side is a parabolic function of  $\langle \Delta \hat{J}_x^2 \rangle$  and for this to be negative requires  $\langle \Delta \hat{J}_x^2 \rangle$  to lie between the two roots of this function, giving

$$\langle \Delta \hat{J}_x^2 \rangle \geq \frac{1}{2} \left\{ \left( J(J+1) - \langle \hat{J}_z \rangle^2 \right) - \sqrt{\left( J(J+1) - \langle \hat{J}_z \rangle^2 \right)^2 - \xi \langle \hat{J}_z \rangle^2} \right\} \quad (304)$$

$$\langle \Delta \hat{J}_x^2 \rangle \leq \frac{1}{2} \left\{ \left( J(J+1) - \langle \hat{J}_z \rangle^2 \right) + \sqrt{\left( J(J+1) - \langle \hat{J}_z \rangle^2 \right)^2 - \xi \langle \hat{J}_z \rangle^2} \right\} \quad (305)$$

which are the required inequalities in Eq. (171) and (172).

## 17 Figure Captions

Figure 1. Bloch vector and spin fluctuations shown for original spin operators.

Figure 2. Regions in the  $\langle \Delta \hat{J}_x^2 \rangle$  versus  $|\langle \hat{J}_z \rangle|$  plane (shown shaded) for states that satisfy (a) the spin squeezing inequality Eq. (173) (b) the smaller Heisenberg uncertainty principle inequality Eq. (171) and (c) the larger HUP inequality Eq. (172). The case shown is for  $J = 1000$  and HUP factor  $\xi = 1$ . Both  $\langle \Delta \hat{J}_x^2 \rangle$  and  $|\langle \hat{J}_z \rangle|$  are in units of  $J$ . The spin operators are chosen so that  $\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0$ .

Figure 3. As in Figure 2, but with  $J = 1000$  and HUP factor  $\xi = 10.0$ .

Figure 3. As in Figure 2, but with  $J = 1$  and HUP factor  $\xi = 10.0$ .

Figure 1:

Figure 2:



Figure 3:

Figure 4:

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